A COMPUTATIONAL FLUID DYNAMIC EVALUATION
OF UNCONFINED HYDROGEN EXPLOSIONS
IN HIGH PRESSURE APPLICATIONS

A Thesis

by

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ABSTRACT

Over the last few decades, the demand for hydrogen has significantly grown. Its high energy content and relatively small environmental effect make it an ideal energy source and chemical feedstock. However, the perceived high risk of hydrogen in the eyes of society is a key challenge that has to be addressed before any future widespread utilization of hydrogen can be achieved. Hydrogen is highly flammable and combustible when mixed with air. It is also very light and buoyant, resulting in a false assumption that hydrogen will not explode in unconfined space. However, there have been at least fourteen industrial incidents involving an unconfined hydrogen vapor cloud explosion (VCE), which show the knowledge gap in hydrogen safety that requires further research.

In this study, the consequences of unconfined hydrogen releases were evaluated using computational fluid dynamic simulation software, FLACS, to determine its potential to explode and to analyze the parameters that can promote hydrogen VCE: initial pressure, time to ignition, and leak height position.

This study concluded that high-pressure hydrogen has the potential to build up a large vapor cloud and explode even without confinement. The highest overpressure produced in the simulation was 0.71 barg, which resulted from igniting a hydrogen gas cloud from a 207 bar hydrogen source leaking at 1 m height. This study also gave the recommended distance from a high-pressure hydrogen processing unit to nearby occupied buildings to use in conjunction with industrial spacing tables for fire hazards.

DEDICATION

In loving memory of my mothers

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CONTRIBUTORS AND FUNDING SOURCES

Contributors

This work was supervised by a thesis committee consisting of Professor Mahmoud El-Halwagi, Professor M. Sam Mannan of the Artie McFerrin Department of Chemical Engineering and Professor Maria A. Barrufet of the Harold Vance Department of Petroleum Engineering.

All work for the thesis was completed independently by the student, under the advisement of Roy Winkler of Citgo Petroleum Company.

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TABLE OF CONTENTS

LIST OF FIGURES

Page

LIST OF TABLES

CHAPTER I

INTRODUCTION

I.1 BACKGROUND

Hydrogen is one of the most widely used chemicals in today's industry. In fact, more than eleven million metric tons of hydrogen were produced annually in United States alone. There has been a large interest in utilizing hydrogen as a base chemical and energy carrier, especially with the global concern of greenhouse gases and depleting fossil fuel reserves. It is an attractive future energy carrier that produces no greenhouse gases and has a dense energy content. In the chemical and refinery industry, hydrogen is used to produce ammonia and methanol, to remove sulfur from fuel, for hydrocracking, and in a surprising variety of other uses, such as food processing.

Despite its versatile use, hydrogen production, handling, and utilization carry many safety hazards. With a wide range of flammable concentration from 4% - 75% and low energy ignition (1/10 of what is needed to ignite gasoline vapor and natural gas), hydrogen has the NFPA 704's highest rating on the flammability scale because it is easy to ignite and even explode. For that reason, it was very important to study hydrogen safety in relation to its flammability and explosive characteristics.

This study focused on hydrogen explosion in an unconfined area. It is generally agreed that hydrogen releases in confined area will result in an explosion, but the potential of external hydrogen releases to lead to explosions has not been widely recognized. Hydrogen has a positive buoyancy, so it is generally assumed that hydrogen would “float away” and there will not be enough confinement for it to develop into an explosion. However, several incidents involving unconfined hydrogen explosions proved that this assumption was not reliable and needed to be studied further. Studying hydrogen behavior in dispersions and explosions is vital for safety investigations for hydrogen application in various industry and in design of safety measurement, preventing accidents and minimizing damage.

I.2 PROBLEM STATEMENT

One problem of hazards study for hydrogen releases in unconfined areas is the uncertainty of whether the releases will result in a fire or an explosion. Therefore, the problem statement of this study will be:

- Given the current knowledge and lessons learned on hydrogen safety, it is desired to determine whether unconfined hydrogen VCE should be considered as credible events.
- What are the recommendations for facility siting and hazard analysis to reduce the chance of explosion in hydrogen storage and transportation?

I.3 OBJECTIVES

This study was carried out to gain a deeper understanding of hydrogen safety, especially on the credibility of unconfined hydrogen explosion events. Based on the aforementioned problems, the objectives of this study were as follow:

- Carry out a 3D CFD modeling of hydrogen releases using FLACS
- Analyze on parameters that promote the intensity of hydrogen VCE
- Provide facility siting recommendations to reduce explosion chance in hydrogen storage and transportation to minimize injury and property damage.

CHAPTER II

LITERATURE STUDY

II.1 EXPLOSION MECHANISM

Flammable materials are chemicals in any form that ignite easily. Most hydrocarbons are ignitable in open air. Hydrogen, which is usually produced from methane, has a wide range of flammable concentrations and a low energy ignition, making it very dangerous and readily ignitable.

Industrial fires and explosions are not a rare phenomenon and result in high consequences. The main damages of fire and explosion are pressure increases, flying fragments, blast waves, and thermal effects [1, 2]. Moreover, various fire and explosion events may result from an ignition, depending on the ignited material, pressure, release rate, and environment [3].

Fire events are typically categorized under three types; jet fire, pool fire, and flash fire. Each event has different characteristics, destruction power, and countermeasures. Jet fire is the most highly recurring type of fire to occur in the oil and gas industry. It occurs from a high-pressure stream of combustible gas or atomized liquid that was ignited soon after it was released. Though very destructive, jet fire is localized and therefore can be managed by keeping high-risk parts minimum and far from other process equipment. Pool fire shares some characteristics of vertical het fires, but it produces less heat. The countermeasures range from preventing flammable liquid to collect and catch fire and to cover the liquid with foam blanket to prevent combustion reactions. When a flammable gas release was not ignited immediately, it will spread and mix with air, forming a flammable vapor cloud. At this point, it can ignite into an explosion (Vapor Cloud Explosion or VCE) or burn into a flash fire. Flash fires have small thermal hazards and negligible overpressure, and thus are unlikely to cause great damage. Though short-lived, flash fire can burn back into a jet fire at the point of release if the fluid stream is not isolated by the time of ignition.

Explosion of combustible vapor occurs under a specific set of conditions and is highly dependent on the environmental conditions, including turbulence-inducing obstacles near the point of release (congested or confined). There are two mechanisms in which an explosion take place; deflagration and detonation. The main difference was the flame speed of each shock reaction. A deflagration was characterized by a subsonic flame speed and low overpressure, while a detonation has a supersonic flame speed and tends to be more destructive. Even though the conditions that could promote a detonation were considered much too extreme to occur in non-pressurized unit operation, the chance of a detonation to take place was not zero, because a deflagration can shift into a detonation, known as the Deflagration to Detonation Transition (DDT).

Despite the many types of fire and explosion, it does not mean that each event is stand-alone. Jet fire and flash fire can ensue from a same loss of containment event, propagating from one type of fire to another. Furthermore, fires and explosions could occur as a consequence of each other. In many industrial incidents, a gas ignition results in a fire before proceeding into an explosion, or vice versa. Studying high-risk process units and modelling their probable ignition events can assist in increasing the safety level of the industry, from determining the safety distance to organizing emergency preparedness and response.

II.2 CASE HISTORY

Hydrogen has found many uses in various industries, such as chemical, oil and gas, and others. In 2010, it was estimated that the total global production of hydrogen was about 50 million tonnes, around half of that quantity was consumed for ammonia production [4]. The three highest industry costumers of hydrogen are shown in Figure II.1.

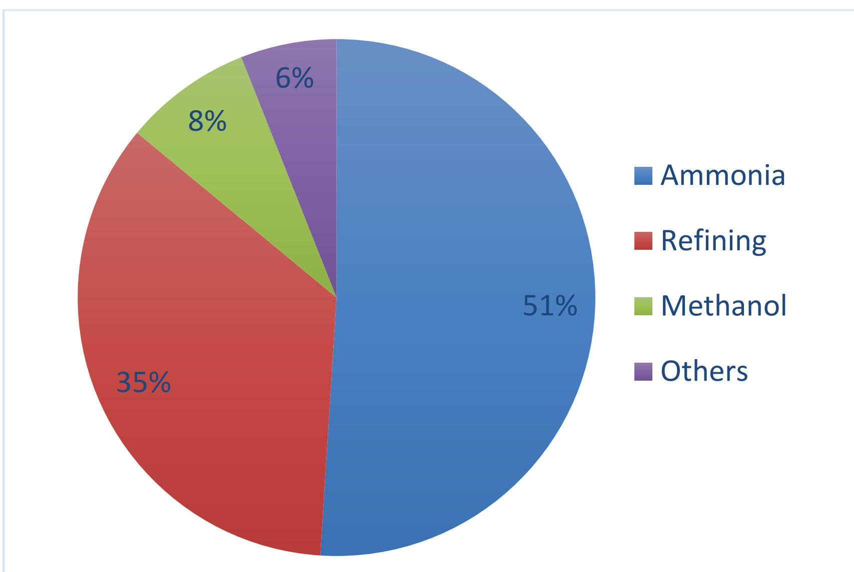

Figure II.1 Hydrogen Consuming Sectors, adapted from [4]

Granted, the more hydrogen an industry uses, the more it is prone to have a hydrogen incident. Zalosh et al compiled all hydrogen incidents in the US in the first half of 1977 and analyzed their findings. Their study reported that hydrogen explosions made up 59% of all reported hydrogen incidents, or more than twice as much as hydrogen fires, as shown by Table II.1 [5]. The highly destructive characteristic of hydrogen explosions also makes it even more troublesome. Around 82% of all casualties in hydrogen incidents had been linked with explosion, as seen in Table II.2. These losses do not include property damage, public insecurity, and loss of production.

Table II.1 Reported Hydrogen Incidents by Industry, adapted from [5]

Industry	**No. of Incidents**	
Chemical	83	30%
Oil Refining	33	12%
Power Plants	30	11%
Metalworking	26	9%
Electronics	19	7%
Food Processing	9	3%
Other or Unidentified	80	29%

Table II.2 Types of Hydrogen Incidents and Casualties Distribution, adapted from [5]

Type of Incident	No. of Incidents		No. of Casualties
Fire	74	26%	8
Explosion	165	59%	63
Pressure Rupture	12	4%	1
Unignited Release	20	7%	1
Fire and Explosion	3	1%	0
Other	6	2%	4

The importance of Zalosh's study was the stark realization of the importance of researching hydrogen explosion mechanisms. It has long been agreed upon that a hydrogen release in an enclosure can result in an explosion, and therefore industries have tried to compensate by placing hydrogen utilization units in unconfined areas. However, the sheer number of hydrogen explosions has proven otherwise.

Until the writing of this thesis, there have been at least 14 incidents involving unconfined hydrogen explosions that provoked many studies and analyses on the credibility of the practice of 'hydrogen only explodes in confined spaces' [6]. Two of the most well-known cases of unconfined hydrogen explosions were Jackass Flats and Polysar Sarnia.

The Jackass Flats incident occurred in 1964 in Nevada and was one of the most studied hydrogen explosions. Los Alamos Scientific Laboratory was testing rocket motor with hydrogen as fuel when a large amount of hydrogen was deliberately released in a congestion-free environment at an initial pressure of 3400 psi and an initial rate of 54.4

kg/s^2 to evaluate the sound pressure levels. After thirteen seconds of testing, approximately 10% of the released hydrogen (around 200 lb) was ignited into a VCE [6]. The explosion was preceded by a fire at the nozzle, believed to be started by electrostatic discharge or mechanical sparks [7]. Blast pressure generated by the explosion could be felt as far as 150 ft at approximately 0.5 psi [7].

The Polysar Sarnia incident occurred in Polysar Petrochemical Complex in Sarnia, Canada. Approximately 65 pounds of hydrogen was released from a compressor's failed gasket. The gas cloud flew into a partially enclosed area and was ignited into a VCE after 10-15 second delay. Window and structural damage was observed as far as 900 m away [8]. Later studies concluded that the extensive damage caused by this incident was due to deflagration-to-detonation transition, or DDT [6].

II.3 FLAME ACCELERATION SIMULATOR (FLACS)

This study was performed by 3D computational fluid dynamic simulations using Flame Acceleration Simulator (FLACS) to simulate hydrogen releases in different environment and the damage of the resulting explosion and/or fire.

FLACS is a computational fluid dynamics (CFD) modelling software that has been developed since 1980 to simulate atmospheric dispersion, fire, and explosion. It was originally intended for offshore modules simulation, but later found more applicable uses in process plant simulations and with a more varying gas or liquid composition. FLACS solves compressible conservation equations on a 3D Cartesian grid using a finite volume method. The key advantage of this software was that it uses distributed porosity to represent geometry and therefore was able to simulate complicated geometries using a Cartesian grid.

Field experiments on hydrogen are not an economic nor a safe approach. Hydrogen is dangerous and expensive to test in a safe environment. The Jackass Flats incident was a hydrogen experiment that was not expected to explode. FLACS can give a full 3D model, and thus can give a more accurate prediction of a chemical dispersion in a certain environment. Other simplified prediction tools for gas dispersion and explosions, while easier and faster to use, lack the ability to model the relevant physics and predict the effects of a certain incident. However, simplified tools may be used for first level investigations and to filter cases that need deeper investigations.

By simulating a possible fire or explosion incident, it was possible to predict future incident consequences to the environment and the effects to human lives and safety. Another benefit for process engineers was that they can design more effective safety and mitigation measures to improve the safety and cost effectiveness of the process unit.

II.4 STATE-OF-THE-ART

Even though the credibility of unconfined hydrogen explosion was still under question, it has invoked several studies regarding the topic, especially after the two aforementioned incidents in chapter II.2 occurred.

Thomas, et al summarized fourteen cases involving unconfined hydrogen explosions, dated from 1964 to 2007 and simulated hydrogen releases using FLACS and SafeSite$_{3G}$®. The discharges took place in the center and on the edges of a typical congested process module in an otherwise unconfined area. The case parameters of the study were rate of release, location of release, and the volume of the resulting flammable cloud. The study concluded that hydrogen's buoyancy, which was thought to be able to promote dispersion in the atmosphere to dissipate the concentration below non-flammable range, does not prevent a flammable mixture to occur in events of high release rates. As such, the combination of moderate levels of congestion and a lean/rich hydrogen mixture was enough to trigger a DDT [6].

Another study on unconfined hydrogen explosions was done by Dorofeev to calculate safe distances to avoid significant blast damages. Computational fluid dynamic simulations require a lot of time and effort, which make simple analytical tools very useful as estimator and screening tools to select cases that require a more complicated and detailed simulation. The study reckoned that the obstacle geometry of the environment in which hydrogen had dispersed has a significant effect on the maximum flame speed of the resulting explosion. However, for very low and very high releases of hydrogen, the effect of congestion becomes negligible. As such, a release of 1000 kg of hydrogen in an obstacle-free environment could result in a deadly situation, and a small release of hydrogen in a confined space was unlikely to result in a combustible mixture [1]. This study emphasized the importance of modelling the probable explosion that can result within a hydrogen unit in a specific environment to determine a safe distance to reduce injuries and damage loss.

A more recent study on unconfined hydrogen explosions experimented and compared CFD simulations with two mathematical methodologies (Eddy Dissipation Concept model and multi-physics combustion model). Tolias et al tested the effects of grid and domain size on the accuracy of the model and found that 1.0 m cell size and domain boundaries the length of 1.875 times of the distance of the further sensor will achieve results with a better agreement with real cases [9].

Even though computational experiments have many advantages over large-scale, open-space experiments (time, cost, facility, and safety), some critical characteristics can only be observed by real-time experiments. Moreover, real-time experiments were necessary to validate the accuracy of computational models. Kim et al experimented on unconfined hydrogen explosions using soap bubble method, and Groethe et al did large-scale hydrogen explosion experiments. Kim et al concluded that lean hydrogen-air mixtures produce explosions with different behavior than rich mixtures, and that flame acceleration highly influences the intensity of blast wave [2]. In one of Groethe's experiments, a combustible hydrogen mixture was released at a high rate in an open-space area and was spontaneously ignited shortly after the initial release [10]. The author did not provide further explanation to this behavior.

CHAPTER III

RESEARCH METHODOLOGY

III.1 METHODOLOGY

The approach method of this study is illustrated in Figure III.1. The data input consisted of control variables and fixed parameters. The control parameters were initial pressures, time to ignition, and leak height position, which will be discussed further in chapter III.2 . Simulation scenario setup would had to be verified initially. The following step was CFD simulation to examine gas cloud distribution and overpressure of possible ignitions. The scenario was simulated as a jet flow of high-pressured hydrogen leaking from a tank in an unconfined environment with no obstruction. The gas cloud was then ignited at certain points where gas cloud VCE was possible. Due to FLACS' limitation in determining boundary conditions, each scenario was split into 2 simulations: dispersion and explosion. Dispersion simulation was executed first to get the hydrogen gas cloud profile and to find the appropriate ignition point that will produce a VCE with the highest overpressure. The second simulation was then conducted by loading the data result from the dispersion simulation into the explosion simulation. The effect of each parameter on the intensity of hydrogen VCE was then analyzed, and conclusions were drawn based on the analysis.

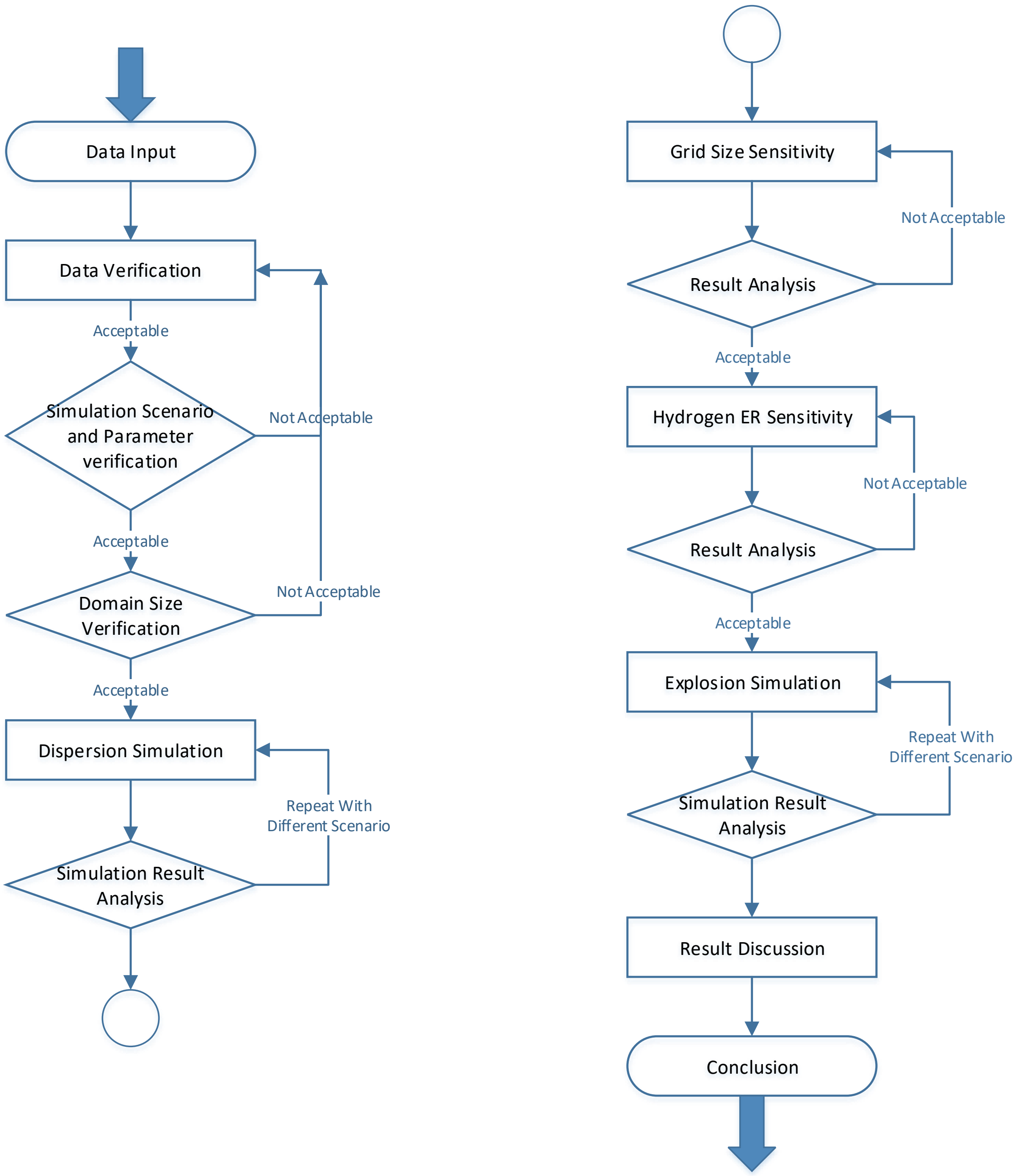

Figure III.1 Research Methodology Flow Chart

This study aims to gain an understanding of possible damages caused by blast overpressure from an unconfined hydrogen explosion without discrediting the fire hazards. Fires and explosions could occur as a consequence of each other. Unconfined hydrogen explosions may be triggered by a flash fire or vice versa. However, this study focused on explosion hazards because the fire hazard of hydrogen releases in unconfined spaces is already widely received and there are several standards and guidelines available for hydrogen fire hazards assessment. The main damages from fire are mostly the heat and flame impingement while the main damages from explosions are overpressure and pressure impulse. In doing facility citing, process engineers should consider both hazards and all possible consequences. Consult appropriate standards such as API 750, 752, 753, 756 to prepare against fire hazards.

III.2 CONTROL PARAMETERS

Several parameters were tested during the CFD simulation to study its effects in promoting unconfined hydrogen explosions:

- Initial pressure
- Time to ignition
- Leak height position

In total, 8 scenarios with different parameters were conducted. A summary of all considered scenarios is presented in Table III.1.

Table III.1 Summary of Simulation Scenarios

No.	Pressure (bar)	Time to Ignition (s)	Leak Height Position (m)
1	69	1	1
2	69	20	1
3	138	1	1
4	138	20	1
5	207	1	1
6	207	1	2
7	207	20	1
8	207	20	2

Initial pressure could not be inputted to FLACS directly, and thus needed to be converted to mass flow rate. Hydrogen gas was released through a small hole into an open space area at approximately 1 atm, hence it could be assumed that the gas was choked at the leak area and the velocity of gas was sonic. Using this assumption, the mass flow rate of hydrogen was calculated by this expression:

$$Q_m = C_0 A P_0 \sqrt{\frac{\gamma g_c M}{R_g T_0}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}} \text{ [11]}$$

Where:

$Q_m = mass\ flow\ rate$

$C_0 = Discharge\ coefficient$ (assumed to be 0.85)

$\gamma = Heat\ capacity\ ratio$

$$R_g = ideal\ gas\ constant$$

For leaks through a 2-inch diameter hole, the hydrogen mass flow rates for each corresponding initial pressure are shown in Table III.2. The calculation for the mass flow rate from 69 bara hydrogen tank is demonstrated in Appendix A.

Table III.2 Hydrogen Mass Flow Rate Through a 2-inch Diameter Hole

P (bar)	**Q_m (kg/s)**
69	6.55
138	13.10
207	19.66

III.3 MODEL DESCRIPTION

Input parameters in FLACS CFD simulations were the geometry/environment, the grid, and the scenario parameters. For the geometry, an open-space area with no obstructions was used. The environment is pictured in Figure III.2, consisting of a horizontal tank on a flat, open terrain. The tank has a length and diameter of 9 m and 3 m, respectively. The terrain itself was 1000 m by 1000 m long to accommodate the hydrogen gas cloud during the dispersion simulation. The vast size was chosen to eliminate the effect of boundaries on the resulting gas cloud.

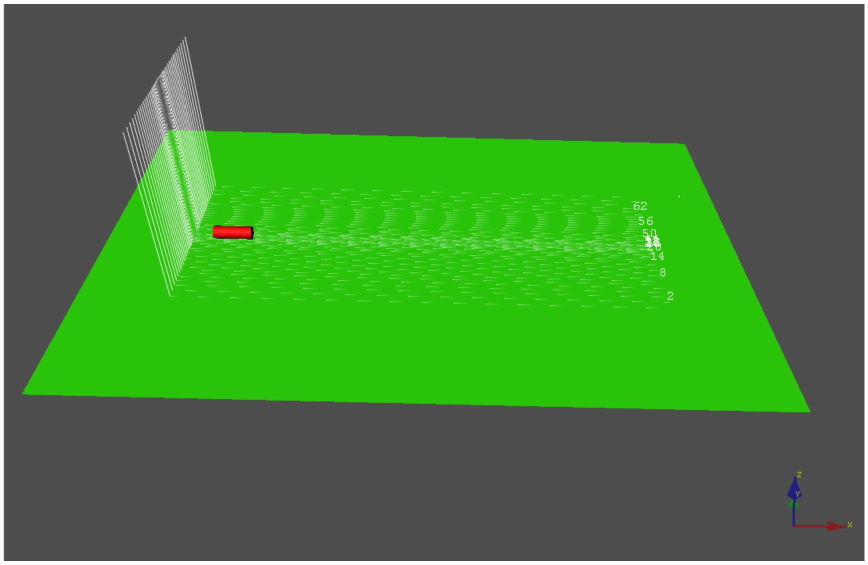

Figure III.2 Open-Space Environment Simulation with a Leaking Tank

The hydrogen was assumed to leak from a hole on the side of the tank, at a height of 1 m or 2 m above the ground. The leak was oriented horizontally along the x-axis toward the open terrain with no obstructions. Figure III.3 shows the position and orientation of the leak.

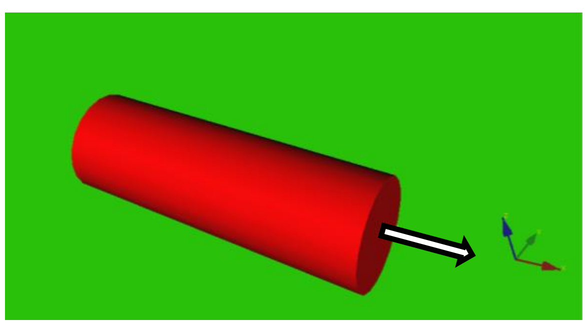

Figure III.3 Position and Orientation of the Leak in an Open-Space Environment

The simulations were divided into 2 stages: simulation of hydrogen dispersion and ignition of the release. First, hydrogen dispersion was simulated to observe the distribution behavior of hydrogen in an unconfined area. From the result, possible time and location of ignitions were selected, and the data was imported into a new domain for an explosion simulation. This approach provides the flexibility to select several ignition times and positions without having to recreate the whole simulation, and to use different boundary conditions for dispersion and explosion simulations.

The timing and location of ignitions were selected by studying the dispersion simulation result. The ignition of the jet cloud was assumed to occur near the ground within the hydrogen's flammability range. In one simulation, the jet cloud was ignited at a time close to the start of the leak with a small but concentrated hydrogen cloud and in another, the jet cloud was ignited at a longer time for a diluted, but more developed hydrogen cloud.

FLACS simulation parameters were inputted according to the user manual. For boundary conditions, this study uses a windy scenario with an atmospheric stability Pasquill class F and 2 m/s wind (common scenario in FLACS hydrogen dispersion research). Wind direction was at 270°, the same direction as that of the leak. The ground was assumed to be an open flat terrain with few obstacles, with roughness at 0.03 m [12].

FLACS uses a Gaussian mesh as the simulation cell. In case of the dispersion simulation, the size of the core cell was set at 1 m, and stretched at a 1.2 stretch factor. The area around the leak was refined to 0.45 m to increase the accuracy of the simulation. The domain size was 300 m by 100 m by 100 m for dispersion simulation. As for the combustion simulation, the domain will be increased to 1000 m by 1000 m by 500 m to prevent overpressure reflections from the boundaries.

For boundary conditions, the Euler and wind boundary were used for the dispersion simulation, while the plane wave boundary was used for the explosion simulation. Plane wave is a non-reflecting boundary condition, chosen to minimize the boundaries' reflection since the scenario is an unconfined area. There would still be some reflection near the boundaries, but it would be minimal because of the extended domain.

III.4 OUTPUT VARIABLES

This study aims to gain a better understanding of hydrogen explosion behaviors in unconfined areas. There were several output parameters on FLACS that can facilitate it. However, FLACS only processes the output parameters that were defined during the scenario setup instead of all parameters, because doing so will make the simulation time too long. Output data can be presented in scalar time graph and 2D graph. Output parameters chosen for the dispersion and combustion simulations are described in Table III.3 and Table III.4, respectively.

Table III.3 Output Parameters for Dispersion Simulations

Parameter	Description
FMOLE	Fuel mole fraction
ER	Equivalence ratio
FUEL	Fuel mass fraction

Table III.4 Output Parameters for Combustion Simulations

Parameter	Description
P	Pressure
PROD	Combustion product mass fraction
MACH	Mach number value
PIMP	Pressure Impulse

CHAPTER IV

RESULTS AND DISCUSSION

IV.1 DISPERSION RESULT

This chapter describes the simulation result of a hydrogen dispersion in an open space environment. The key parameters to be analyzed from the dispersion simulation result are the hydrogen dispersion profile and the extent of the flammable cloud encompassing the Lower Flammability Limit (LFL), which is an important consideration to set distances between hydrogen process/reservoir units with occupied buildings or hazardous zones (electrical, fire hazards, or hot work zones).

Figure IV.2 shows the concentration profile of a hydrogen dispersion twenty seconds after the start of the leak. The initial pressure was 207 bar and the height of leak was 1 m. The common argument is that a hydrogen gas leak in an unconfined area will rise and disperse relatively quickly due to the buoyancy, and therefore does not have a significant VCE risk. However, this profile shows that this is not always the case. A large hydrogen release rate has a significantly high momentum, which dominates the flow close to the source point more than the buoyancy force during the initial time of release [6]. The buoyancy force in the dispersion simulation only started to take effect at the end of the gas cloud, signified by the upward bending of the gas cloud, where the source pressure was weakened due to the distance.

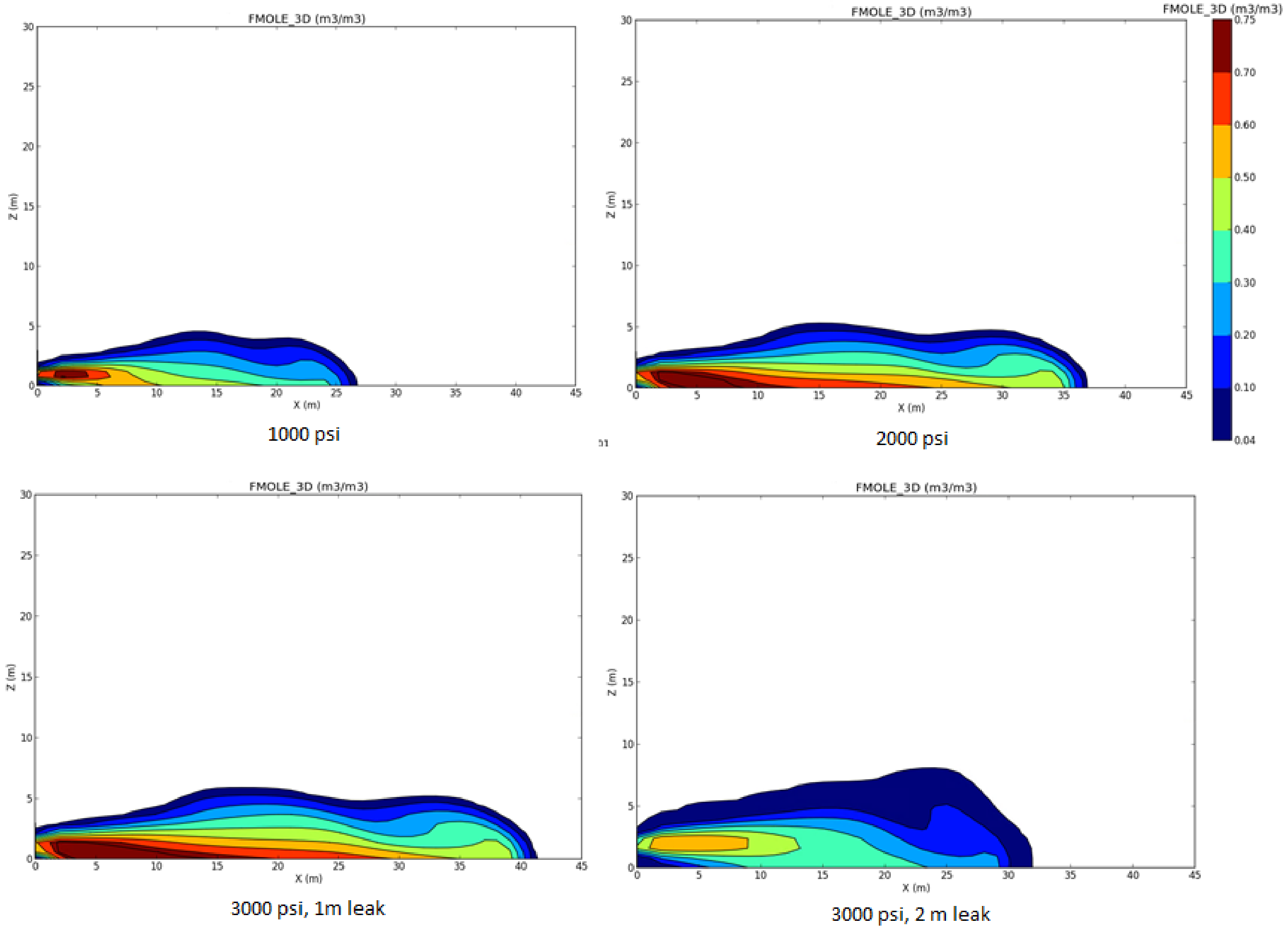

Figure IV.1 Hydrogen Concentration Profile 1 Seconds after the Start of Leak

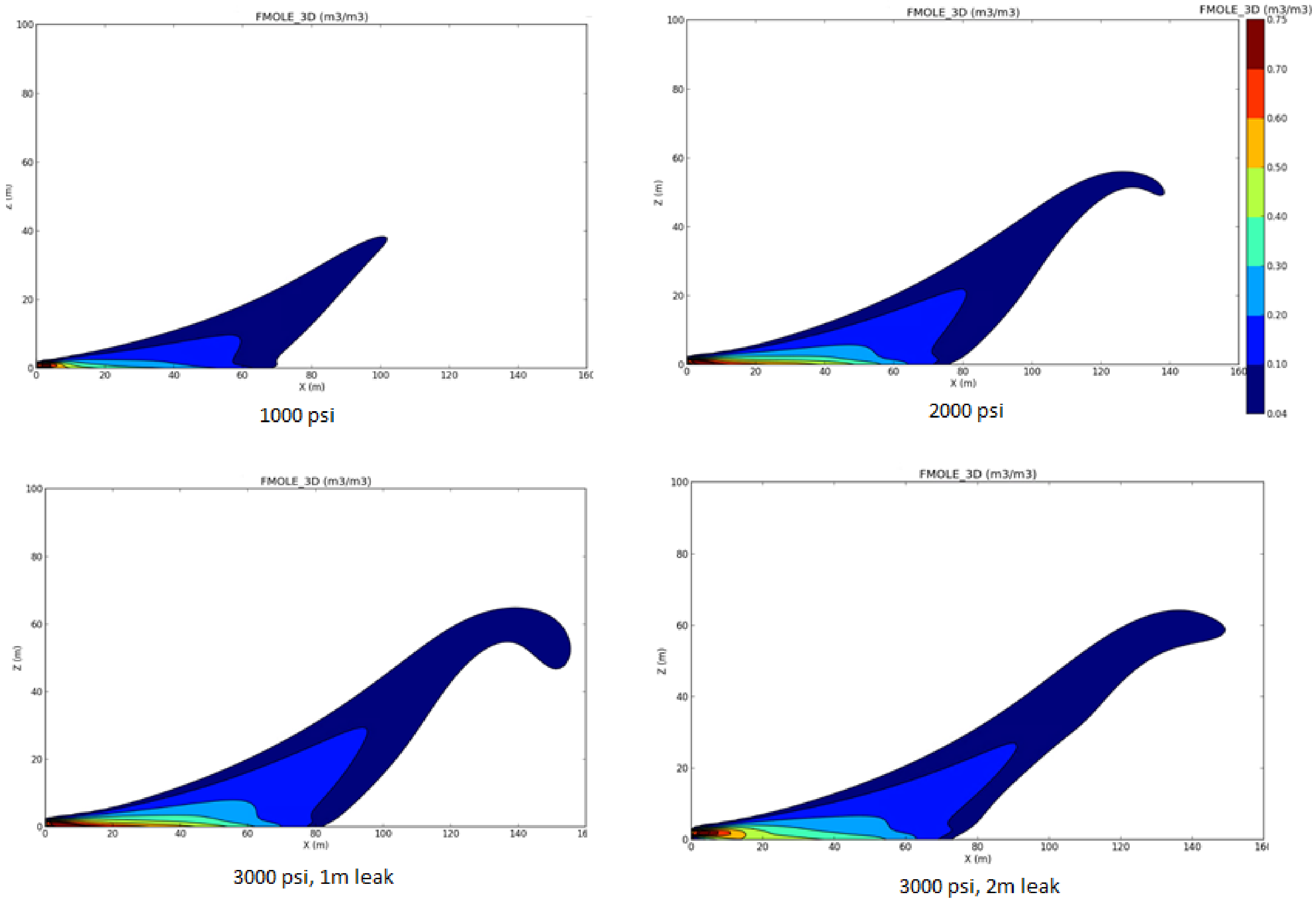

Figure IV.2 Hydrogen Concentration Profile 20 Seconds after the Start of Leak

The hydrogen concentration profiles in Figure IV.2 were shown for the flammable range only (4% to 75%). For the hydrogen release at 207 bar and 1 m leak, the distance to the lower flammability limit (LFL) was more than 150 meter from the release point, and the gas cloud did not 'lift' (signifying the strong buoyancy force of hydrogen taking effect) until around 80 m. In fact, even at an initial pressure of 69 bar, gas cloud did not lift until 70 m.

Table IV.1 Gas Cloud Characteristics at Different Parameters

No.	Initial Pressure (bar)	Leak Height (m)	Distance Before Gas Cloud Begins to 'Lift' (m)	Max. Gas Cloud Volume (m3)
1	69	1	70	320
2	138	1	75	830
3	207	1	82	1490
4	207	2	72	1460
5	207	10	-	1170

Table IV.1 shows the characteristics of hydrogen gas clouds with different initial pressure and leak height. As expected, a higher initial pressure produces higher momentum that 'pushes' the jet stream and prevents hydrogen buoyancy force from taking effect and lift it. Therefore, the higher the initial pressure of hydrogen leak, the longer it takes before the gas cloud can lift. This poses a bigger risk with high pressure hydrogen, since the longer the hydrogen gas cloud stays near the ground, the higher its possibility to get in contact with an ignition source and ignite.

Another point of interest here was the distance of the release point to the ground. In their paper, Bénard et al argued that when the leak was close to the ground, the LFL extent of the gas cloud would increase along the direction of the leak [13]. At an initial pressure of 207 bar, when the leak position was moved higher to 2 m, hydrogen was quicker to disperse with air and lift off the ground. In fact, the distance for the cloud to lift was less than the one with a lower initial pressure. Figure IV.2 shows how hydrogen gas disperses as a function of leak height. However, the size of the gas cloud itself remains roughly the same.

The increase in the extension of the flammable cloud caused by the presence of a surface relatively close to the jet centerline can be explained by a phenomenon called the Coandă effect. The Coandă effect is described as “the tendency of a jet of fluid emerging from an orifice to follow an adjacent flat or curved surface and to entrain fluid from the surroundings so that a region of lower pressure develops” [14].

A free jet of fluid will mix with its surrounding as it flows away from the leak source. However, when the jet is close to a surface, it results in a pressure reduction across the jet and a reduced entrainment on the side of the jet facing the surface. This causes a suction pressure in the area between the jet and the surface, and so the jet is deflected closer to the surface, clinging itself to it. [13]. With such a condition, the region between the jet and the surface cannot provide enough air for the entrainment. This explains the stretched LFL extent of the hydrogen gas cloud in Figure IV.2.

As comparison, a concentration profile of a free jet-flow hydrogen is shown in Figure IV.3. The initial pressure was 207 bar, and the leak was located at 10 m to cancel out the Coandă effect from the ground. The gas cloud only reached 130 m as compared to 160 m when the leak was at 1 m. It also took less time for hydrogen to disperse, as there was more air available for entrainment.

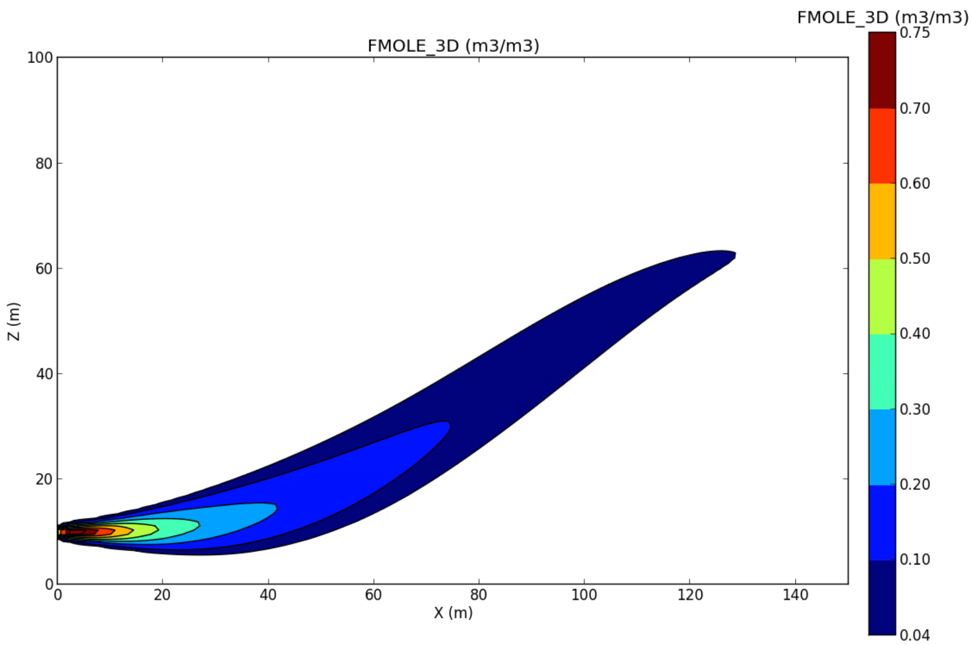

Figure IV.3 Hydrogen Concentration Profile at 207 bar Initial Pressure and 10 m Leak Height

The influence of Coandă effect on hydrogen jet flow dispersion has been confirmed by field experiments [15, 16]. Therefore, it can be concluded that the closer the leak source was to the ground, the longer the jet will cling to the ground. This is important to mention during hydrogen hazard study because most of the simplified techniques to calculate hydrogen safe distances are based on a free flow jet.

With the momentum force and the Coandă effect delaying hydrogen dispersion and extending the gas cloud LFL reach, it is clear now that with a high initial pressure and release rate, a hydrogen release can produce a significant and concentrated gas cloud even without a confinement.

IV.2 GRID SIZE SENSITIVITY

In CFD simulations, grid cells must be sufficiently small to produce an accurate numerical result. However, the number of grid cells will be exponentially larger with very small grid size, and thus will be impractical to simulate. There has not been any widely applied methodology for grid sensitivity other than a few guideline from FLACS-GexCon. Consequently, a grid sensitivity analysis was performed to have better confidence in the results. Through this analysis, it was desired to see the effect of the grid size on the simulation and to find an appropriate grid cell size for the explosion simulation that will produce an accurate result without expending on simulation time and computer memory.

Analysis was performed with hydrogen dispersion at 207 bar and 1 m. leak height. Grid sizes ranged from 2.5 m to 1 m. The simulation with 1 m grid size produced 2.7 million grid cells and consequently took a long time and a large amount of computer memory to simulate. However, the result was not significantly different from the one with 1.5 m grid size (Table IV.2). Because the maximum overpressure expected from this study will be approximately less than 0.5 barg, explosion simulation in chapter IV.3 and chapter 0will be performed with 1.5 m grid size.

Table IV.2 Grid Size Dependency

Grid size (m)	Max Overpressure (barg)	Difference
2.5	0.21	40.0%
2	0.35	23.9%
1.5	0.46	6.1%
1	0.49	-

IV.3 HYDROGEN CONCENTRATION SENSITIVITY

As hydrogen leaks from the source, it will disperse and mix with air. Therefore, the gas cloud will have different concentrations at different points within the cloud. According to several study, hydrogen's concentration at the ignition point will affect the intensity of the explosion. Even though any gas cloud mixture of fuel and air within its flammability range has the potential to ignite, it does not always produce a pressure wave high enough to be a significant risk, especially when there is no physical obstruction that confines the gas cloud. However, several studies have indicated that the flame speed of the gas cloud has a major effect of the intensity of the hydrogen explosion's pressure wave. A hydrogen gas cloud with a stronger flame speed results in an explosion with a higher peak overpressure than the one with a lower flame speed [2, 17]

Flame speed is described as the propagation velocity of the flame front with respect to a fixed observer, or a sum of the burning velocity and the gas flow velocity [7]. Burning velocity is similar to flame speed, but the velocity of the flame front is calculated with respect to unburned gas. Burning velocity depends on the type of gas involved in the explosion and the gas concentration relative to the oxygen concentration in air. Equivalence Ratio (ER) is a good parameter to measure it. ER itself is defined as follows:

$$ER = \theta = \frac{\left({}^{m_{fuel}}/{}_{m_{oxygen}}\right)_{actual}}{\left({}^{m_{fuel}}/{}_{m_{oxygen}}\right)_{stoichiometric}}$$

Hydrogen has one of the highest burning velocities when compared to other types of fuel. To show the worst-case scenario of an unconfined hydrogen explosion, the gas cloud in this study would be ignited at a point where the ER was expected to produce the highest overpressure. However, the effect of ER on peak overpressure was acquired through a field test, and different test and methodologies could produce different values of ER. Moreover, most of the test was done on a confined space, and therefore was quite different from this study.

The hydrogen concentration sensitivity test was conducted to find the appropriate point with an ER that will produce the highest overpressure possible within a gas cloud. The value of the ER tested was obtained from different studies and shown on Table IV.3. It was to be noted that only Richardson, Skinner et al did their study under unconfined conditions. The rest of the study were confined explosions, and the simulations using their suggested ER produced explosions with low overpressure. The hydrogen concentration that resulted in an explosion with the highest overpressure was 70%, as suggested by Richardson, Skinner et al. Therefore, explosion simulations in Chapter 0will be conducted by igniting the gas cloud at the concentration of 70%.

Table IV.3 Hydrogen Concentration Sensitivity Test

ER	**Hydrogen Concentration (v/v)**	**Source**	**Max Overpressure (barg)**
gas leak point		-	did not ignite
10	75%	-	0.44
5.8	70%	[19]	0.47
5.1	67%	[19]	0.47
1.6	40%	[20-22]	0.31
1.4	36%	[23]	0.26

IV.4 EXPLOSION RESULT

The maximum overpressures for all explosion simulations are presented in Figure IV.4. At the same initial gas pressure, the blast wave overpressure of explosions with one second ignition time were slightly higher than the ones with twenty seconds ignition time. Increasing the height of the leak lowered the maximum overpressure of the explosion. At a 2 m leak height, the overpressure decreased by around 20% compared to the explosion from a 1 m leak height.

At one second after the leak, even though there was only a relatively small amount of flammable gas clouds, it is more concentrated and more reactive. As shown in chapter

IV.3 hydrogen concentration at the point of ignition plays a big role in determining the overpressure of the blast wave. Hydrogen concentration that produces the highest overpressure is around 70%, which is relatively high and difficult to maintain as hydrogen quickly disperses in open air. Right after the start of leak, hydrogen has yet to disperse, and is mostly high-concentrated, hence the higher blast wave overpressure.

Looking at the relatively low overpressure, it was determined that the hydrogen VCE in the simulations were propagated by deflagration. The flame front propagation in deflagration is strongly influenced by turbulence ahead of the flame front, which can either be from the jet flow or interactions with obstacles. In the simulations there were minimal obstructions other than the ground; therefore, the turbulence was mostly from the jet flow of the hydrogen leak. Higher pressure creates more turbulence in the gas cloud, which explains why the blast overpressure is always higher with the increasing initial pressure [7].

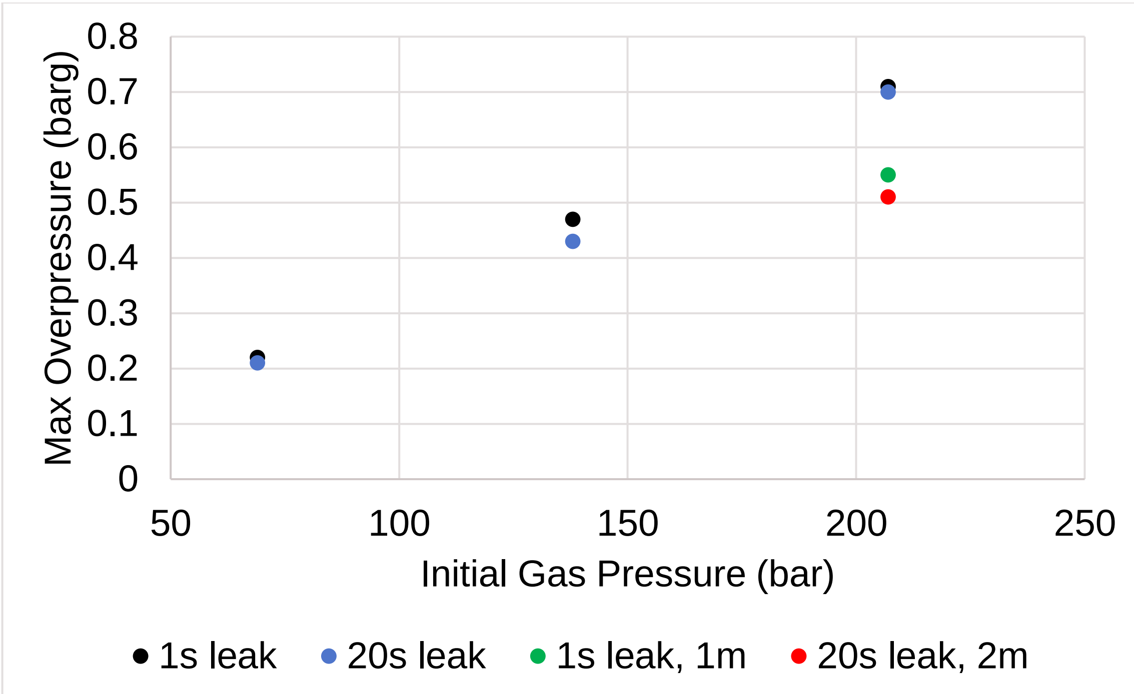

Figure IV.4 Maximum Blast Overpressure as a Function of Initial Hydrogen Pressure and Time of Ignition

Table IV.5 shows the recommended distances for different criteria of buildings from hydrogen units. The first column is for a permanent building, followed by a portable building. Despite the strong structure, many permanent buildings are equipped with windows, which typically start to break around a 0.01 barg overpressure [24]. However, permanent buildings located near covered process areas such as control rooms and operator shelters are typically constructed to be blast resistant and therefore can withstand a much higher overpressure.

Conventional, windowless portable buildings can typically withstand up to 0.04 barg overpressure without experiencing a widespread damage. Studs on the wall facing the explosion are expected to crack but remain in place. However, glass breakage and falling overhead items are expected, and can cause injuries to personnel inside the building [25]. If portable buildings are needed within a location closer than the distance recommended by Table IV.5, it is advised to use a reinforced portable building to minimize damage to personnel. Several commercial portable buildings can withstand up to a 0.5 barg overpressure.

Table IV.4 Maximum Allowable Overpressure for Different Types of Building and on Human Body

Type of Building	**Max Allowable Overpressure (barg)**	**Details**
Permanent building	0.02	Probability 0.95 of no serious damage below this value; 10% window glass broken [26]
Portable buildings	0.04	Max. overpressure for light wood trailers. Reinforced trailers may experience higher overpressure before breaking [25]
Personnel	0.35	Threshold for probability 0.01 of eardrum rupture [27]

The human body can withstand a much higher overpressure than buildings. The threshold for eardrum rupture is as high as 0.35 barg and the threshold for lung damage is 0.83 barg [11]. However, past incidents show that during explosions, personnel are more susceptible to injuries from structural failures, collapsing buildings, debris, and projectiles rather than the direct overpressure itself [26].

Table IV.5 Hydrogen VCE Damages and Recommended Distances

Initial Pressure (bar)	Leak Height (m)	Time to ignition (s)	Ignition position (m)	Max Overpressure (barg)	Max Pressure Impulse (kPa.s)	Distance from Hydrogen Units (m)	
						Permanent Building	Portable Buildings
69	1	1	4	0.22	0.6	58	40
69	1	20	4	0.21	0.6	60	45
138	1	1	6	0.47	0.9	60	60
138	1	20	6	0.43	0.9	115	80
207	1	1	8	0.71	1.2	60	55
207	1	20	8	0.7	1.4	140	120
207	2	1	7.5	0.55	1.3	50	50
207	2	20	7.5	0.51	1.3	125	120

IV.5 DETONATION TO DEFLAGRATION TRANSITION

Without confinement, a hydrogen VCE will most likely have a reaction front slower than the speed of sound (deflagration) and thus causes a relatively small damage. However, hydrogen is highly reactive and it is possible for the deflagration to evolve into a detonation. This phenomenon is called a deflagration to detonation transition (DDT). Detonation has higher, large-scale hazards because the overpressure in a detonation front is much more severe.

The possible occurrence of DDT is rarely mentioned in HAZOP or risk studies. Several facility siting standards such as API RP 752 and API RP 753 do not mention DDT nor consider it as a credible event, despite several industrial incidents involving DDT. The Polysar Sarnia incident mentioned in chapter II.2 was a hydrogen DDT. Several large scale gas VCE experiments where DDT were observed have also been reported [28]

The behavior of DDT is largely still being researched. What is currently understood is that DDT is a phenomenon in ignitable mixtures of a flammable gas and air (or oxygen) where a sudden transition takes place from a deflagration type of explosion to a detonation type. The transition is promoted by the acceleration and merging of the deflagration shock front caused by expanding burned gases and compressive heating effects resulting from the auto-ignition of preheated unreacted mixtures [29]. Deflagration needs turbulence ahead of the flame front (from flow or obstacle interaction), but detonation is propagated by shock-wave interaction (not dependent on obstacle interaction) and can auto-ignite the unburnt gas. During the transition, a volume of pre-compressed, turbulent gas ahead of the flame front detonates at an unusually high velocity and overpressure. Shock waves will ignite unburned gas ahead and lead to much faster flame propagation (1500-2000 m/s) and a higher peak overpressure. Deflagrations are normally less than 10 barg, while detonation shock front can be between 16-20 barg, not including reflection.

FLACS can only simulate deflagrations and therefore cannot predict the consequence of a DDT. However, it has a novel system that can predict the possibility of DDT occurring during a deflagration. The likelihood of DDT is illustrated by two parameters; the spatial pressure gradient across the flame front (DPDX) and the ratio of geometric length scale in FLACS with the detonation cell size (DDTLS). DPDX can indicate when the flame front captures the pressure front, which signifies the start of a DDT. The DPDX value range and its qualitative possibility is shown in Table IV.6.

Table IV.6 DPDX Value Range and the Possibility of DDT, adapted from [29]

DPDX Value	**DDT Possibility**
< 0.5	DDT is not considered likely
0.5 < DPDX < 1	DDT begins to be possible if hot-spot region in flame front was significant
1 < DPDX < 5	DDT is possible if hot-spot region in flame front was significant
DPDX >5	DDT is likely to happen

DDTLS is a parameter that compares the geometric length scale in FLACS with the detonation cell size. The flame front has to cover a large enough area for a detonation to occur. DDTLS with a value of 7 and larger ensures that the initiated detonation front will propagate with enough fuel. In an unconfined scenario, it translates to a stoichiometric gas mixture layer of at least four meters (13 feet) [28, 29].

To analyze the possibility of DDT in this study, two FLACS DDT simulations were conducted with an initial pressure of 207 bar and a leak height of 1 m. The minimal number of simulations is because this is the most extreme condition in which hydrogen is most likely to detonate. The simulation result shows that there is no significant risk of DDT in this case. All DPDX values in the gas cloud are smaller than 0.5. The reason may be the minimal obstruction and how fast hydrogen disperses.

Middha and Hansen (2008) predicted that in unconfined scenario, it needs a stoichiometric gas mixture layer of at least four meters thick for DDT to propagate. In a totally open space area with no obstruction, it won't be possible to have a stoichiometric hydrogen-air mixture that thick away from the ignition point. However, with some kind of obstruction (e.g. wall, obstructed process units, trees, or mounds) DDT may be possible. Therefore, hydrogen facility units should be kept as uncongested as possible. Open space hydrogen VCE involving DDT has happened before, and thus it is possible to occur in hydrogen-consuming industries. Industries should evaluate their facilities for DDT risk and minimize the risk by layout changes or with mitigation methods.

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

V.1 CONCLUSIONS

This study demonstrated a CFD simulation of high-pressure hydrogen releases, in an open space environment, using FLACS to assess the possibility of hydrogen VCE, in an unconfined area. Parameters including the initial gas pressure, the time to ignition, and the distance of leak source to the ground were investigated. The main conclusions are listed below:

- Hydrogen buoyancy does not prevent the formation of a large flammable gas cloud for high-pressure releases near the ground.
- Distance to LFL, in the hydrogen flammable gas cloud, increases the closer the leak source is to the ground.
- Distance to LFL, in the hydrogen flammable gas cloud, increases with higher initial gas pressure and release rate.
- A short time to ignition results in a slightly higher overpressure, even with less hydrogen mass.
- Explosions with a short time to ignition result in a more localized explosion as there is less gas turbulence ahead of the shock front for it to propagate further.
- A minimal obstruction is needed for a hydrogen DDT to occur.

Based on the conclusions of this study, the following recommendations are proposed for hydrogen producers and users:

- Hydrogen facilities should be kept as uncongested as possible and away from ignition sources in order to minimize fire and explosion hazards and to prevent deflagration evolving into a detonation.
- Unconfined hydrogen releases have the potential of leading to an explosion, and therefore should be seriously considered during hazard studies and facility siting.

V.2 RECOMMENDATIONS FOR FUTURE WORK

This study faced some limitations and challenges that the writer believes should be further explored in future studies regarding unconfined hydrogen explosions, such as:

- Explore process design modifications of high pressure hydrogen processing units to increase the inherent safety factor.
- Investigating effects of other parameters on promoting unconfined hydrogen explosions, such as wind speed and direction.
- Carrying out field tests and simulation developments on detonations. Most of the explosion field experiments were on deflagration and thus could not give an accurate estimation of DDT.
- Study of propagation from a hydrogen fire to an explosion.

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APPENDIX A

HYDROGEN LEAK MASS FLOW CALCULATION

This calculation was for the scenario with 69 bar and 200°F hydrogen leaking through a 2-inch diameter hole.

Scenario parameter:

Table A. 1 Calculation Parameters for Hydrogen

Parameter	Description	Value
P	Initial pressure within process unit	69 bar
T	Initial temperature within process unit	200 °F
D_{hole}	Hole diameter	2-inch
C_0	Discharge coefficient	0.85
γ	Heat capacity ratio	1.41
M	Molecular weight	$2\ {}^{lbm}/_{lbmol}$
R_g	Ideal gas constant	$1545\ {}^{ft.lbf}/_{lbmol.°R}$
g_c	Gravity	$32.17\ {}^{ft.lbm}/_{lbf.s^2}$

A.1. Calculating the choked pressure.

The choked pressure (P_{choked}) was the pressure that ensues maximum gas flow rate through a hole. For downstream pressure less than choked pressure, the gas velocity at the leak was the velocity of sound and cannot be increased further [11].

$$P_{choked} = \left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma}{\gamma-1}} * P$$

$$= \left(\frac{2}{1.41 + 1}\right)^{\frac{1.41}{1.41-1}} * 1000$$

$$= 534.3 \; psia$$

Since hydrogen was leaked to atmospheric pressure, which was less than the choked pressure, it can be assumed that the flow was choked and maximized through the leak.

A.2. Calculating hydrogen flow rate:

$$A = \frac{1}{4} * \pi * D^2$$

$$= \frac{1}{4} * \pi * 2^2$$

$$= 3.14 \; in^2 = 0.02 \; ft^2$$

$$Q_m = C_0 A P_0 \sqrt{\frac{\gamma g_c M}{R_g T_0}\left(\frac{2}{\gamma + 1}\right)^{\frac{\gamma+1}{\gamma-1}}}$$

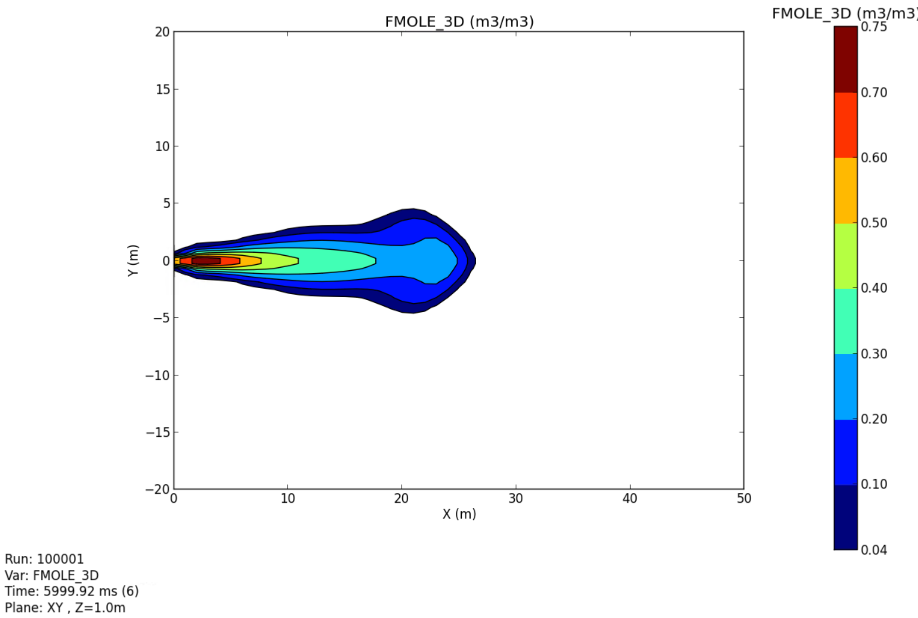
$$= \ 0.85 * 0.02 * 1000 * \ \sqrt{\frac{1.41 * 32..17 * 2}{1545 * (200 + 460)} * \left(\frac{2}{1.41 + 1}\right)^{\frac{1.41+1}{1.41-1}}}$$

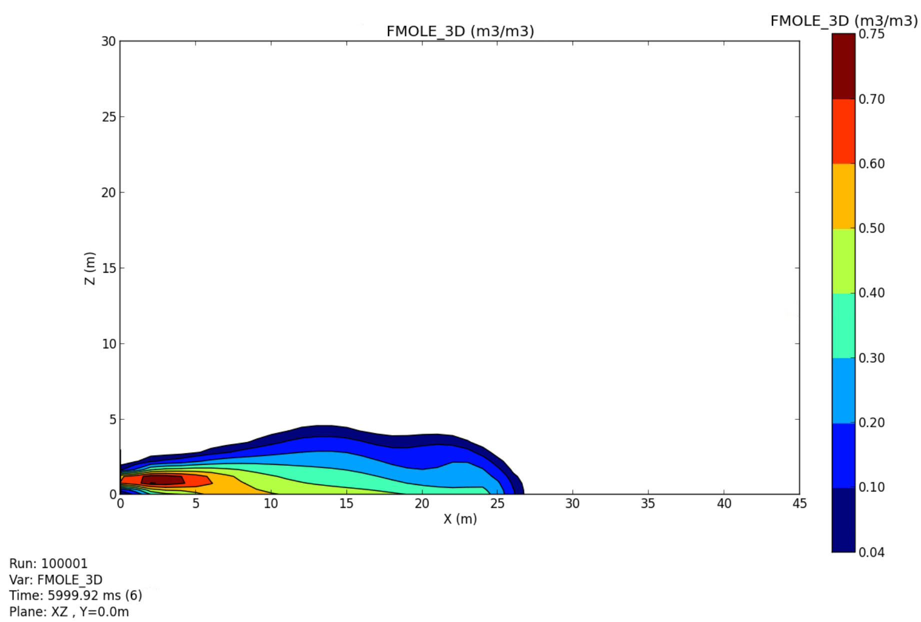
$$= 14.56 \ {}^{lbm}/_{s} = 6.55 \ {}^{kg}/_{s}$$

APPENDIX B

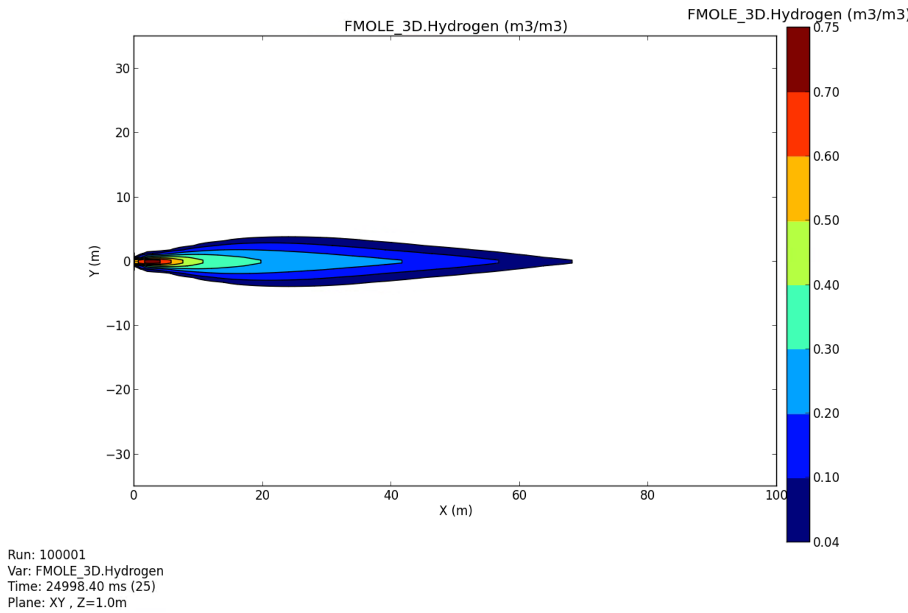
HYDROGEN DISPERSION PROFILE

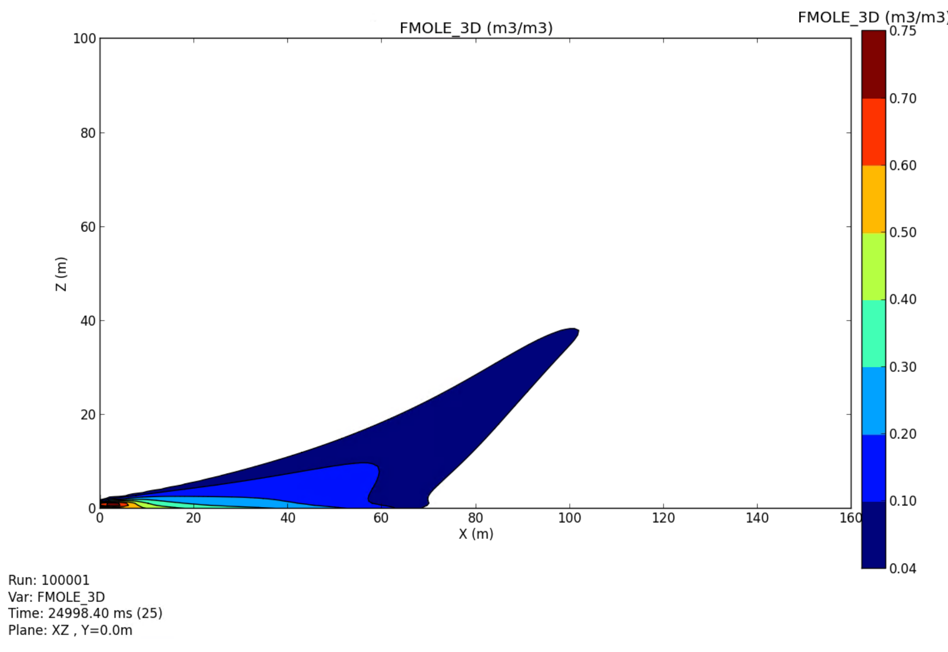
B.1. 69 bar, 1 Seconds



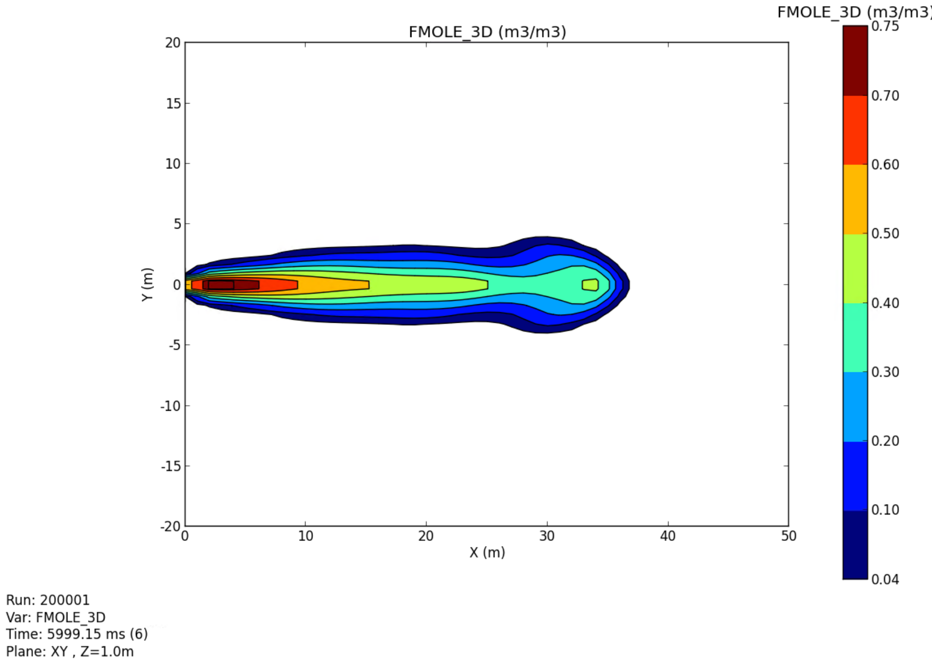


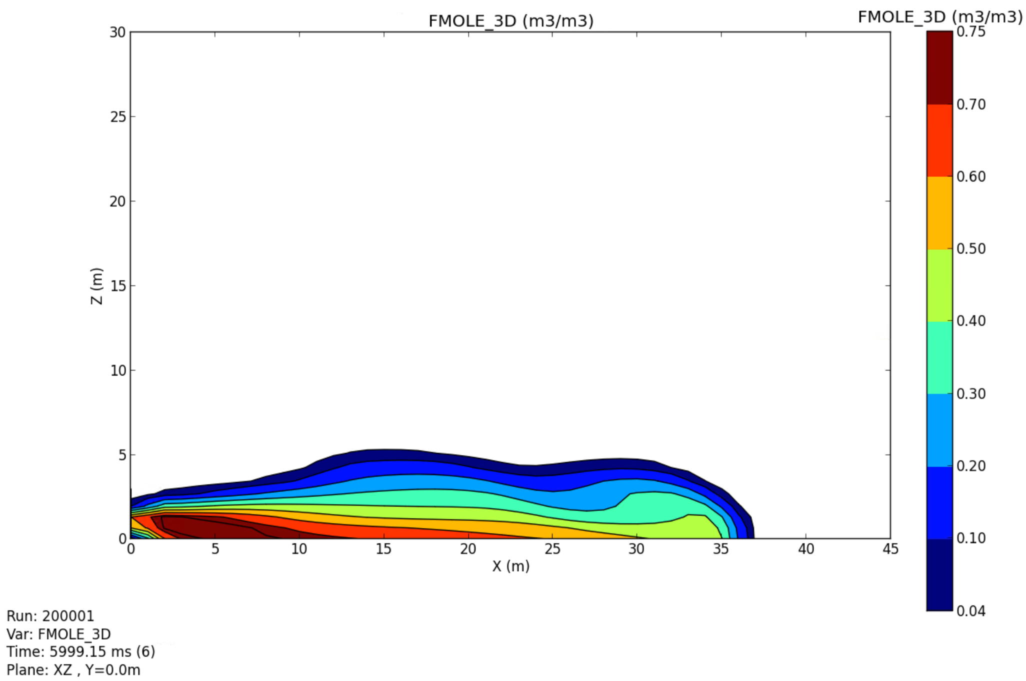
B.2. 69 bar, 20 Seconds



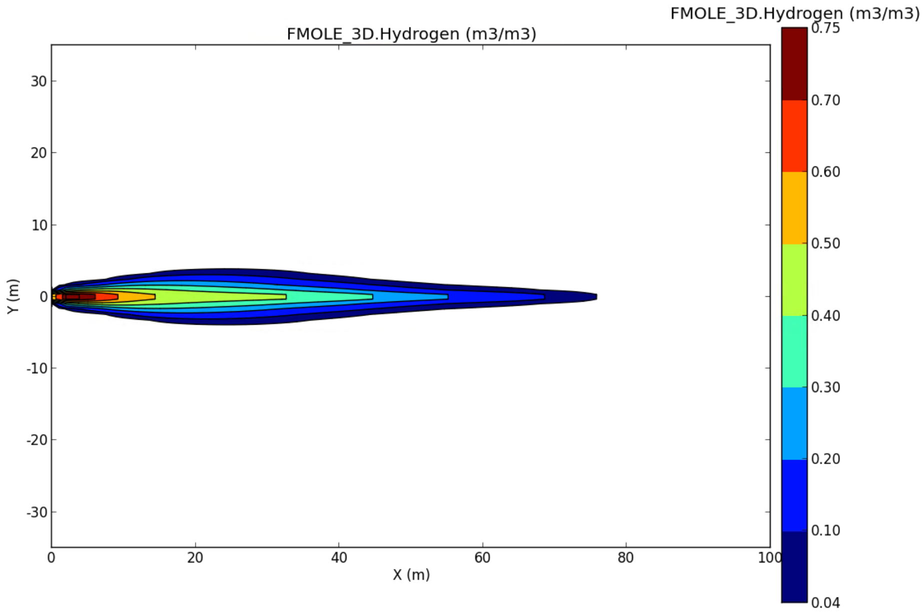


B.3. 138 bar, 1 Seconds





B.4. 138 bar, 20 Seconds



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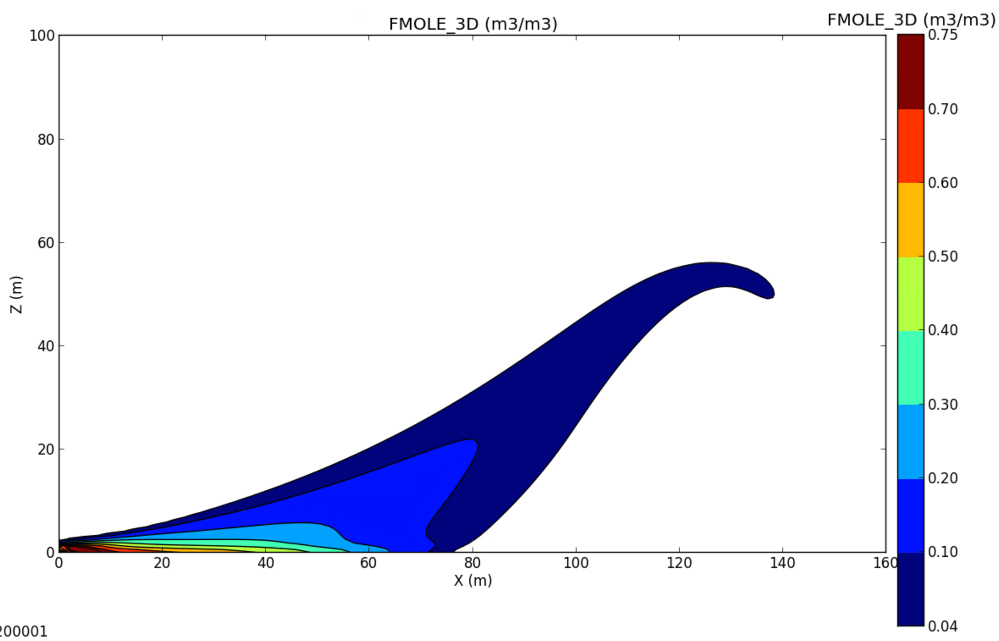
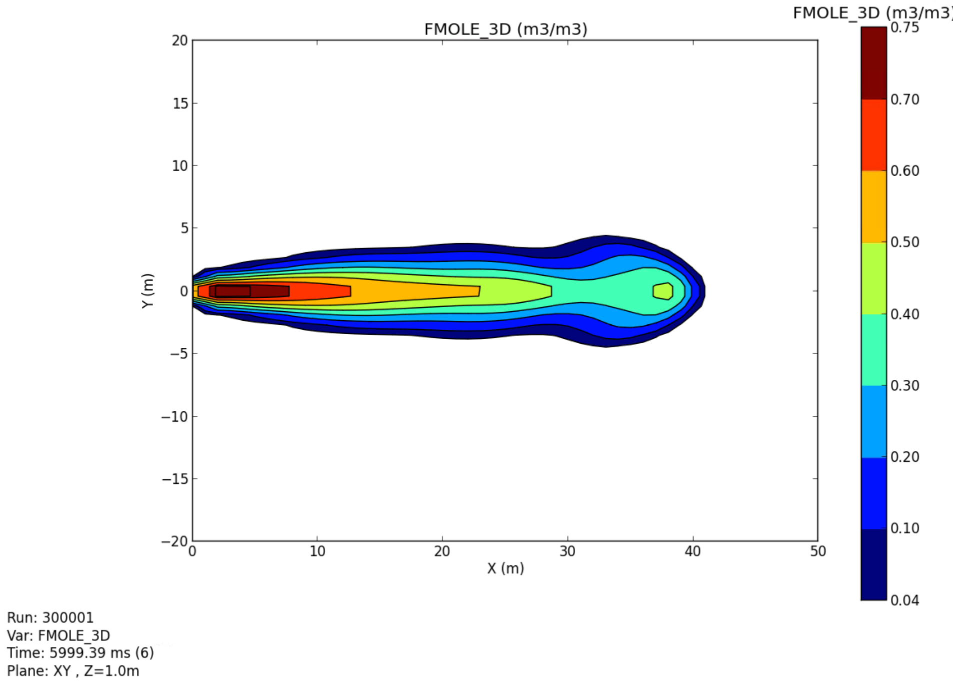
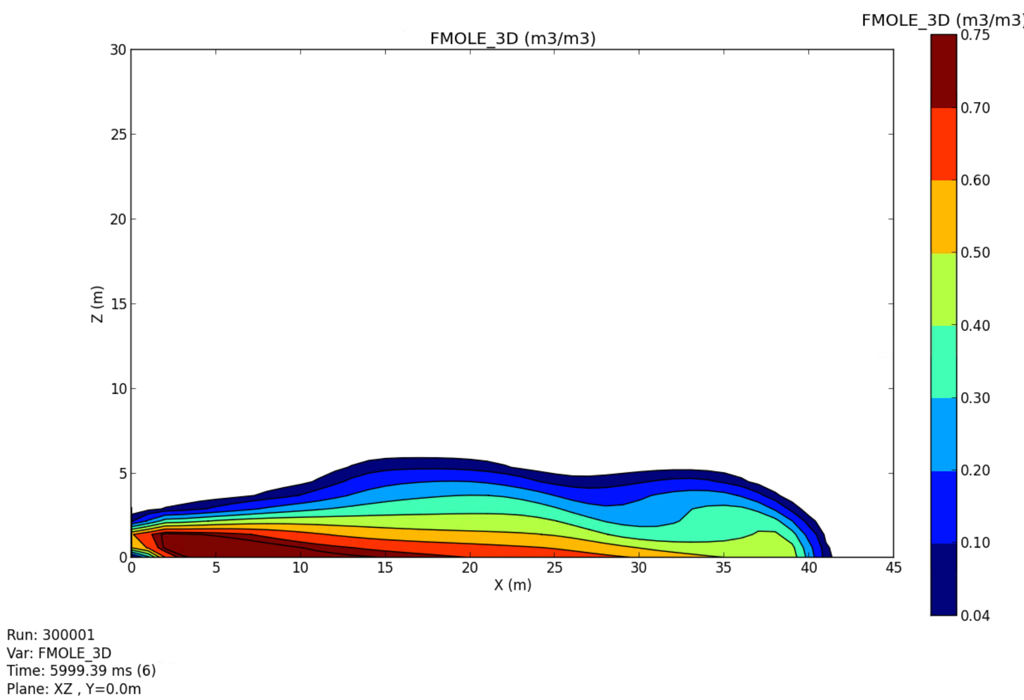
Plane: XY , Z=1.0m



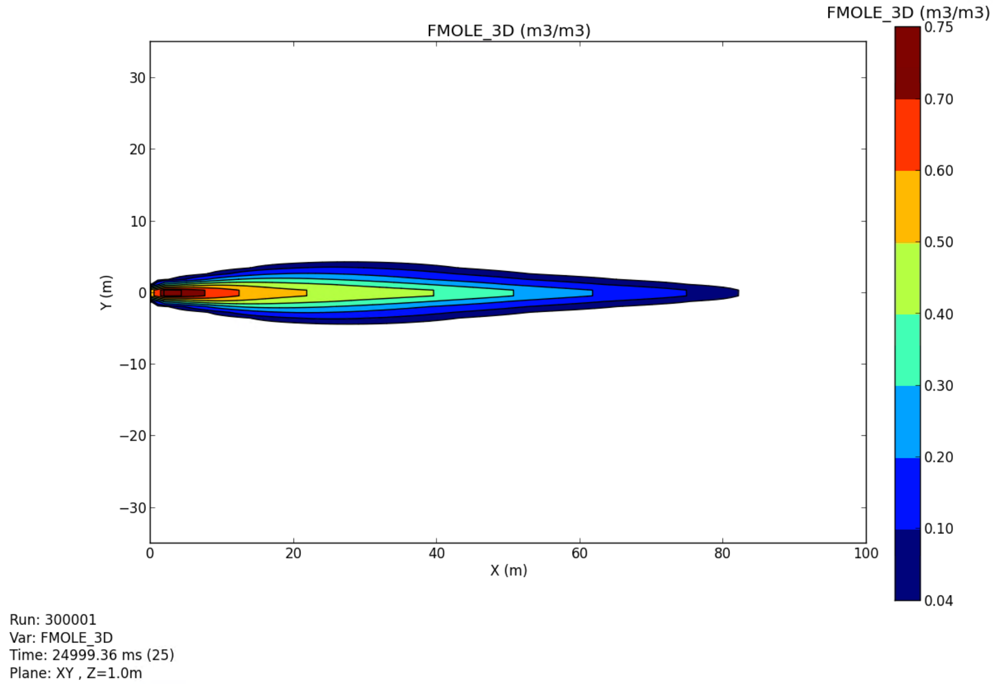
Run: 200001
Var: FMOLE_3D
Time: 24998.01 ms (25)
Plane: XZ , Y=0.0m

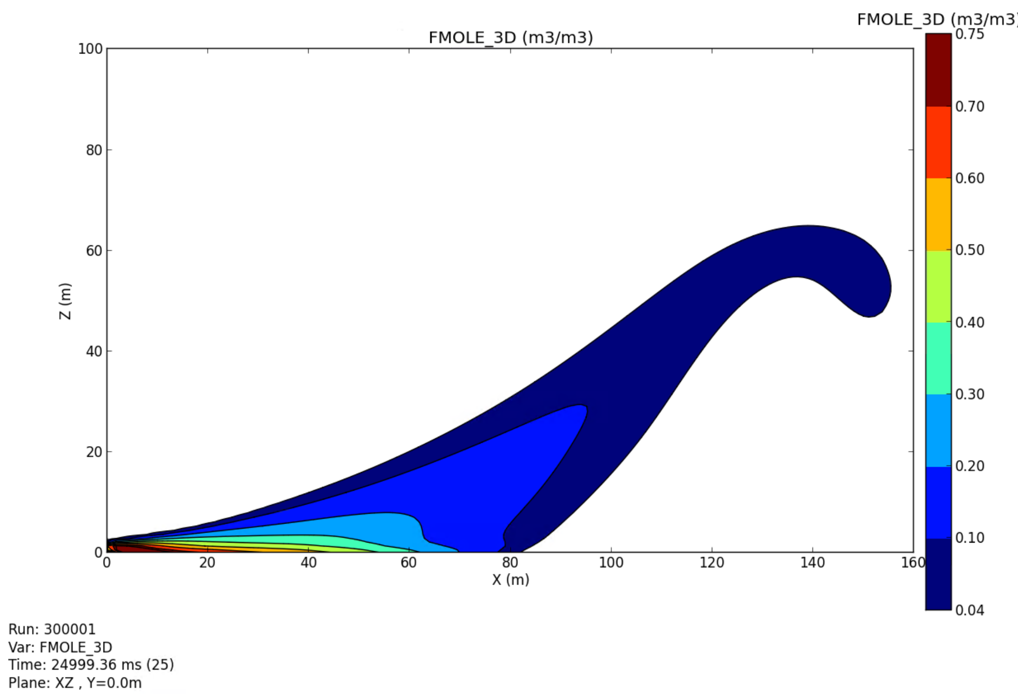
B.5. 207 bar at 1m Height, 1 Seconds



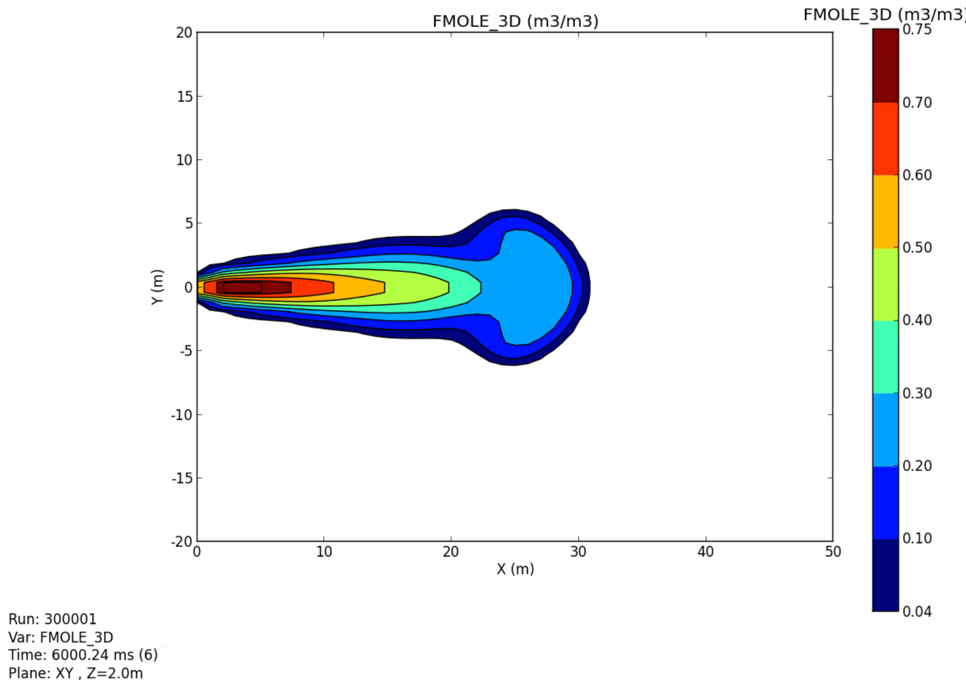


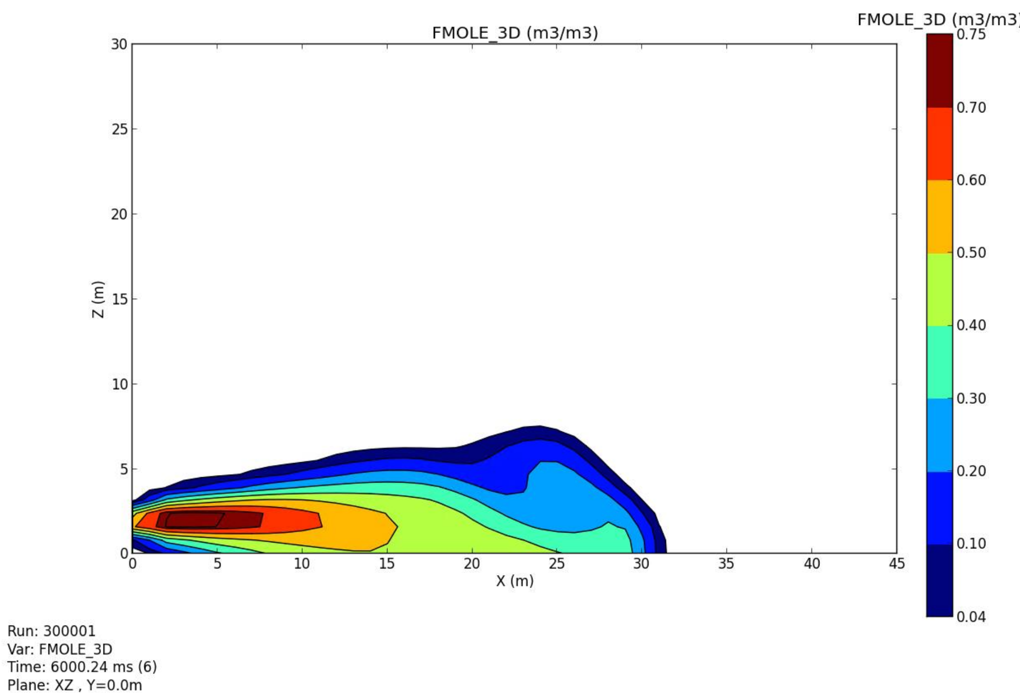
B.6. 207 bar at 1m Height, 20 Seconds



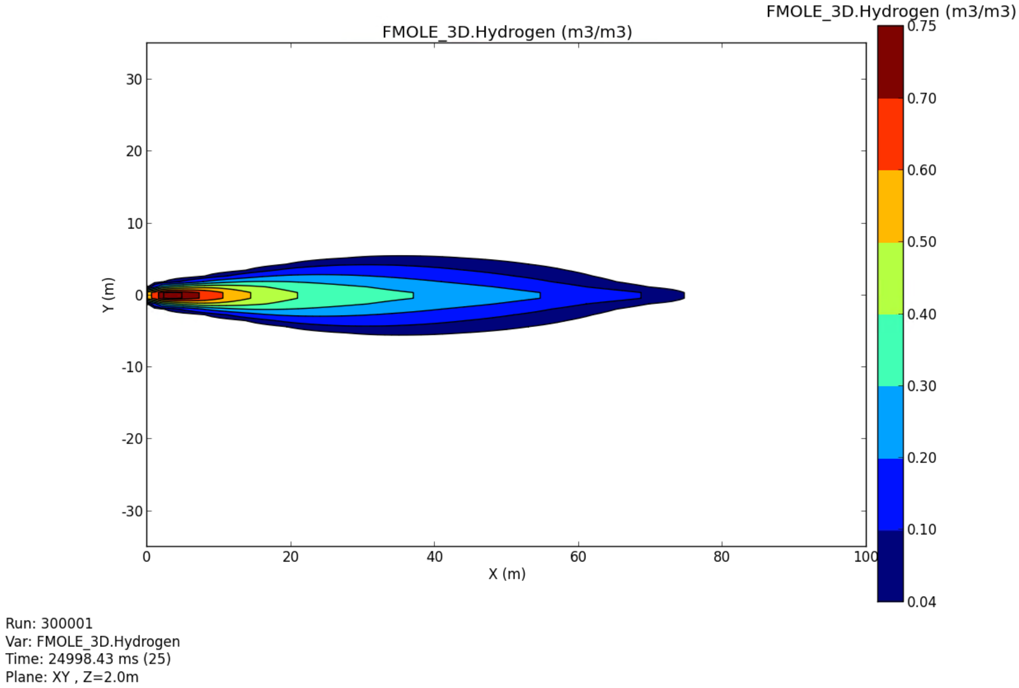


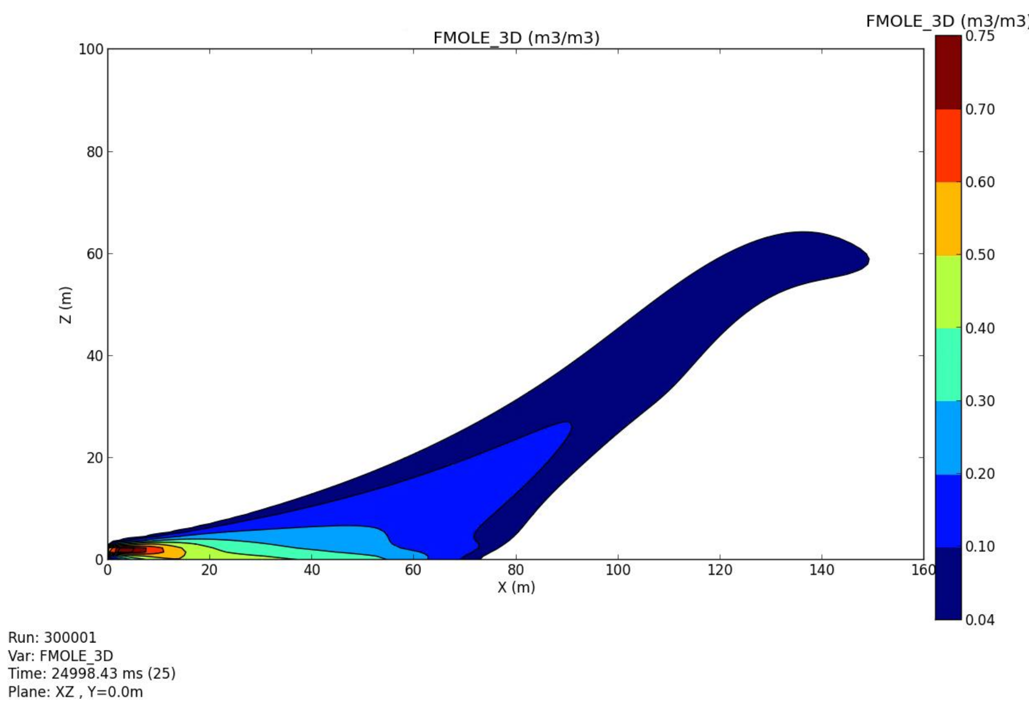
B.7. 207 bar at 2 m Height, 1 Seconds



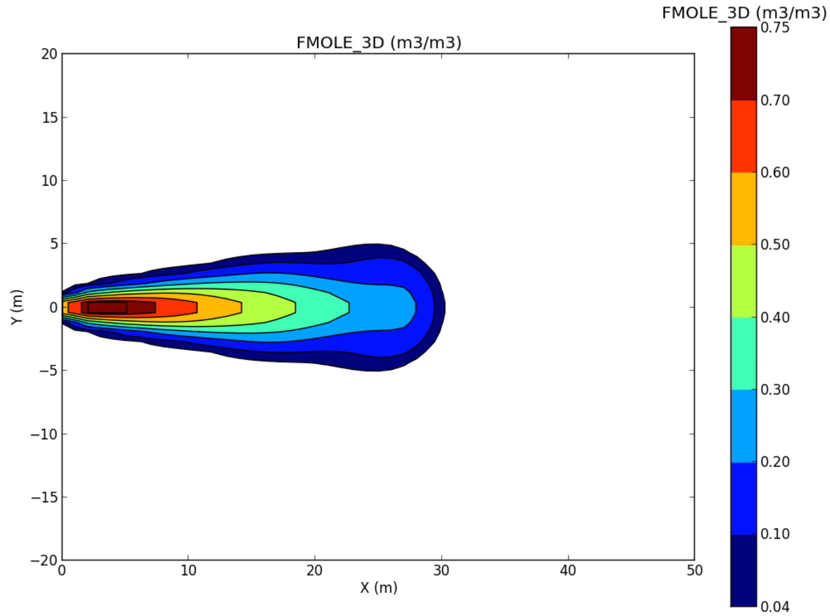


B.8. 207 bar at 2 m Height, 20 Seconds





B.9. 207 bar at 10 m Height, 1 Seconds



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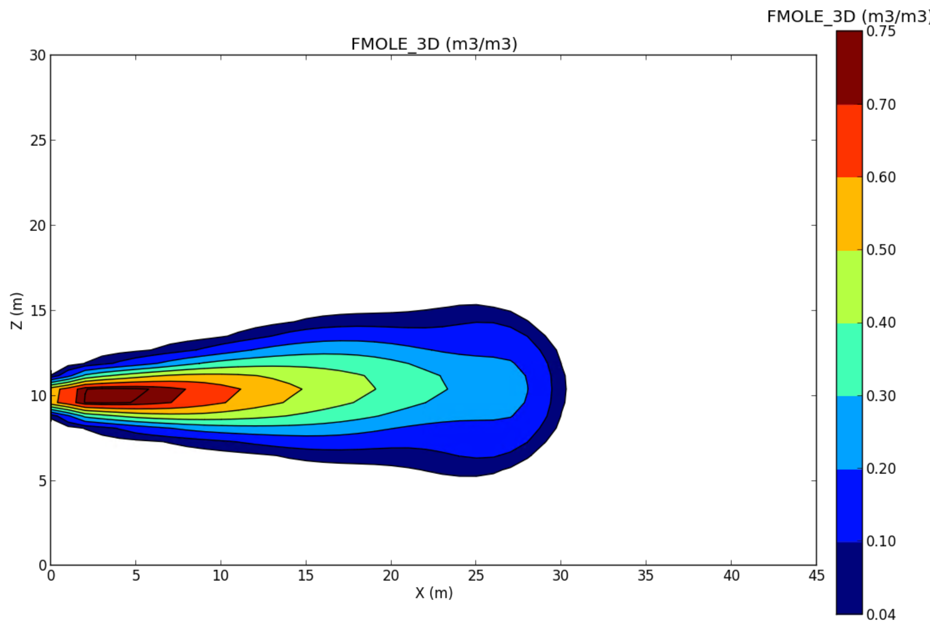
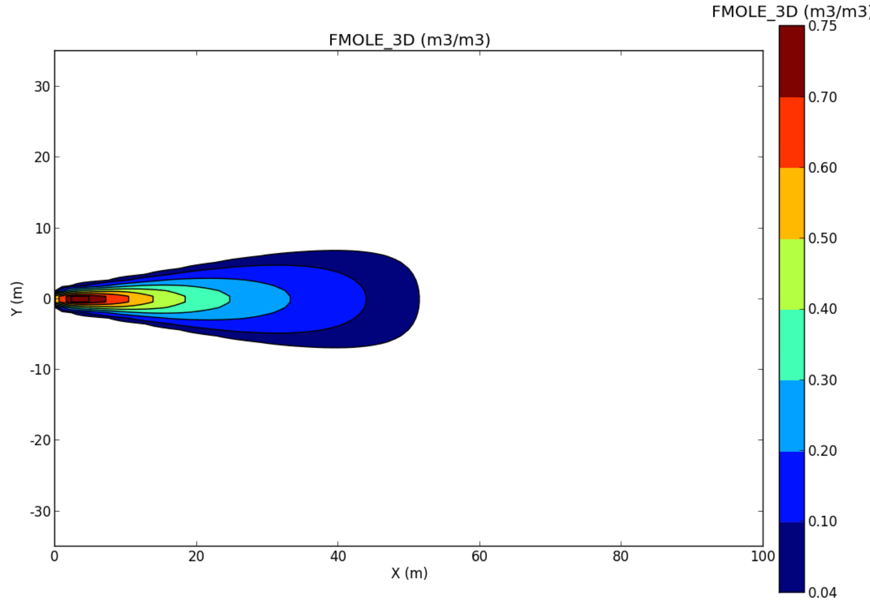
Plane: XY , Z=10.0m

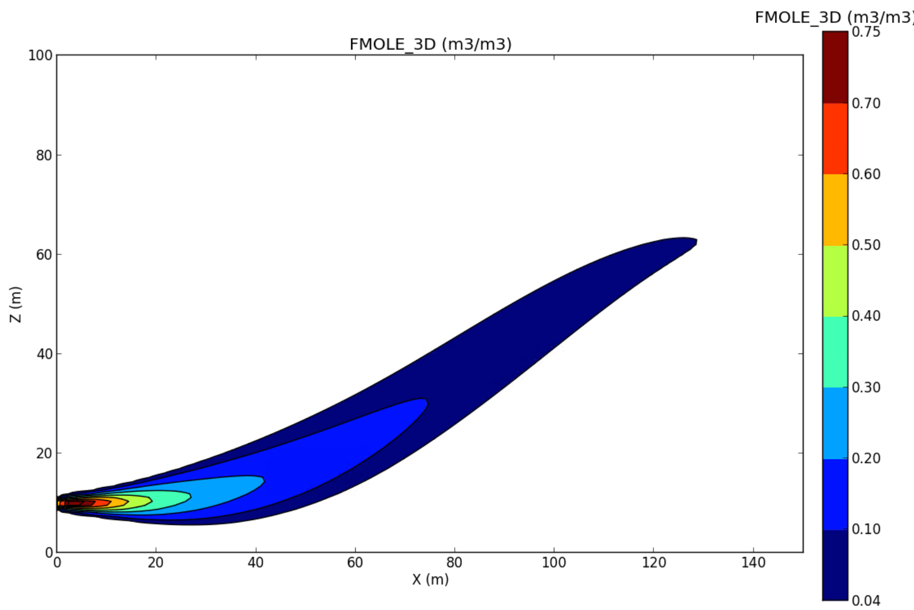


Run: 300002
Var: FMOLE_3D
Time: 6001.76 ms (6)
Plane: XZ , Y=0.0m

B.10. 207 bar at 10 m Height, 20 Seconds



Run: 300002
Var: FMOLE_3D
Time: 24999.57 ms (25)
Plane: XY , Z=10.0m

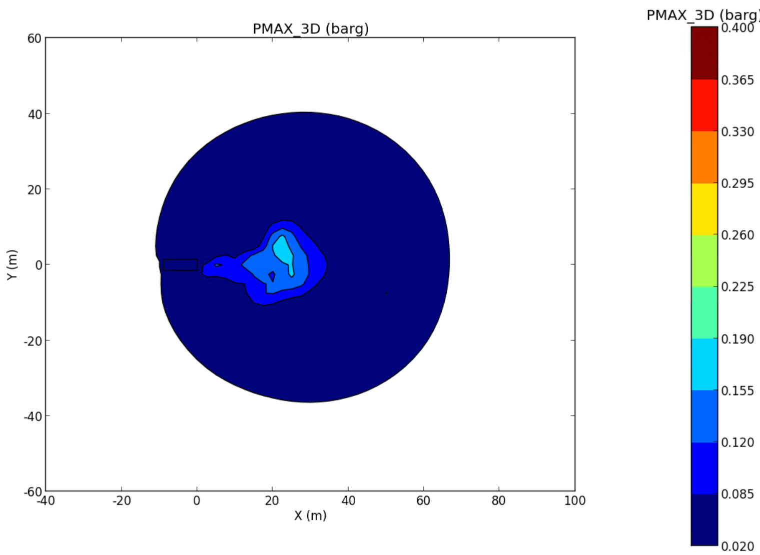


Run: 300002
Var: FMOLE_3D
Time: 24999.57 ms (25)
Plane: XZ , Y=0.0m

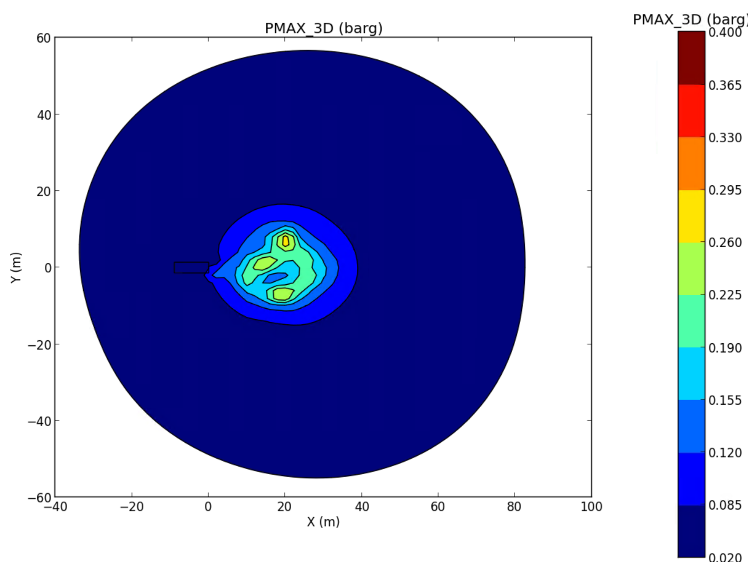
APPENDIX C

GRID SIZE SENSITIVITY TEST

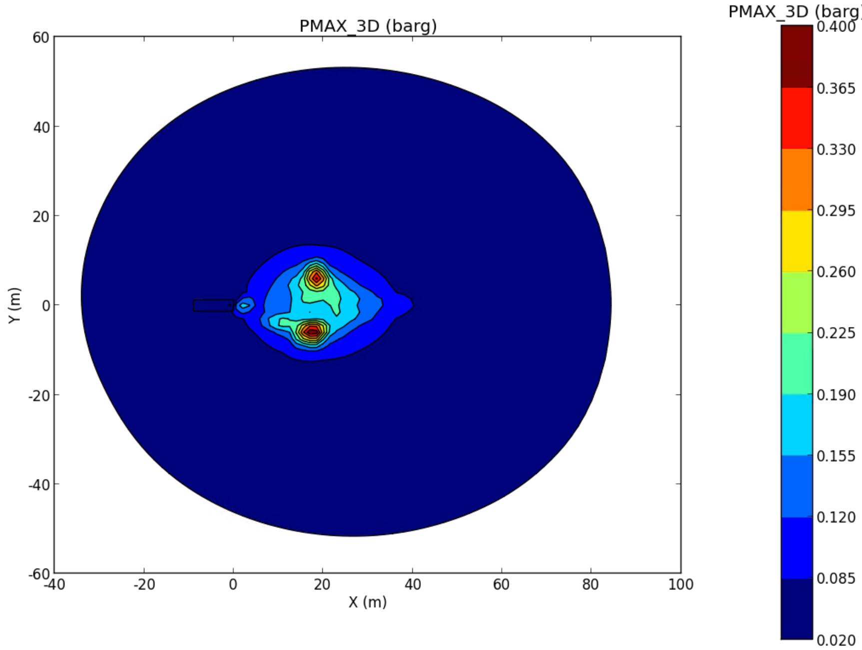
C.1. Explosion Profile with Grid Size: 2.5 m



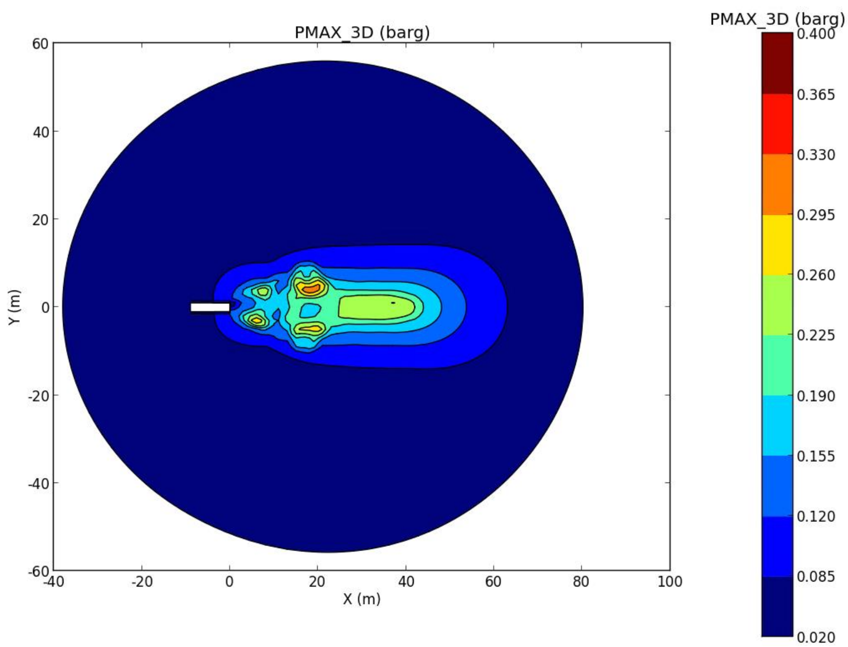
C.2. Explosion Profile with Grid Size: 2 m



C.3. Explosion Profile with Grid Size: 1.5 m



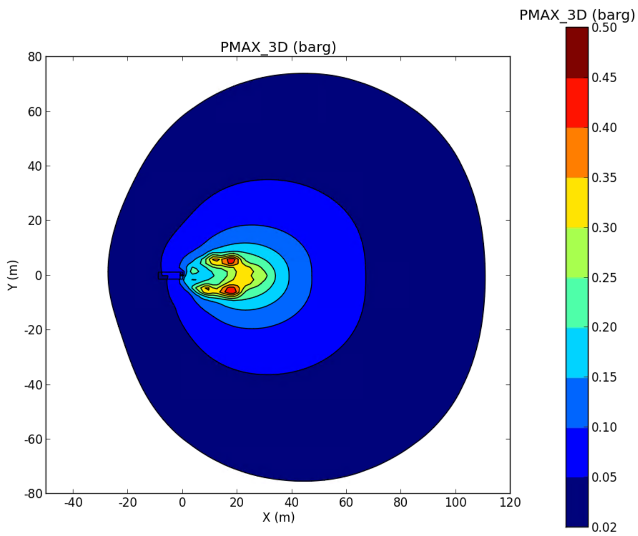
C.4. Explosion Profile with Grid Size: 1 m



APPENDIX D

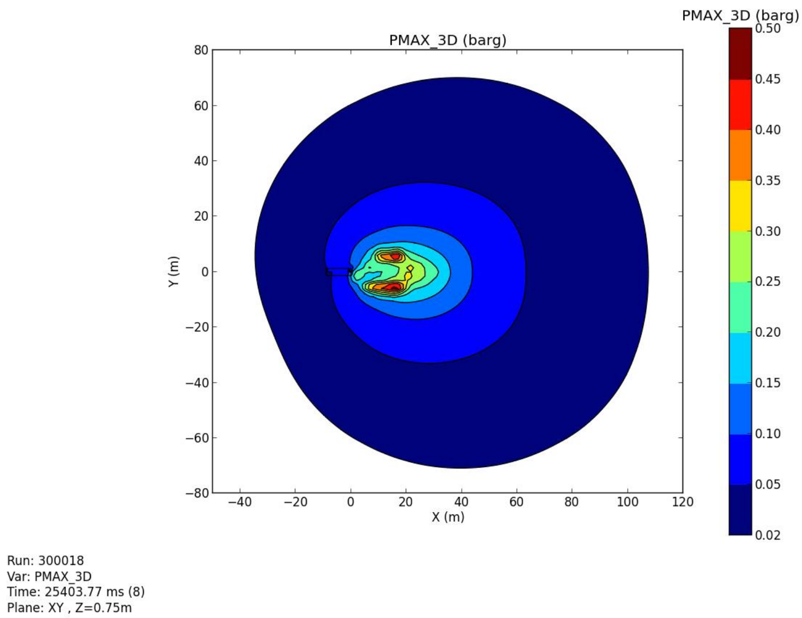
HYDROGEN CONCENTRATION SENSITIVITY TEST

D.1. Explosion Profile at Hydrogen Concentration: 75%

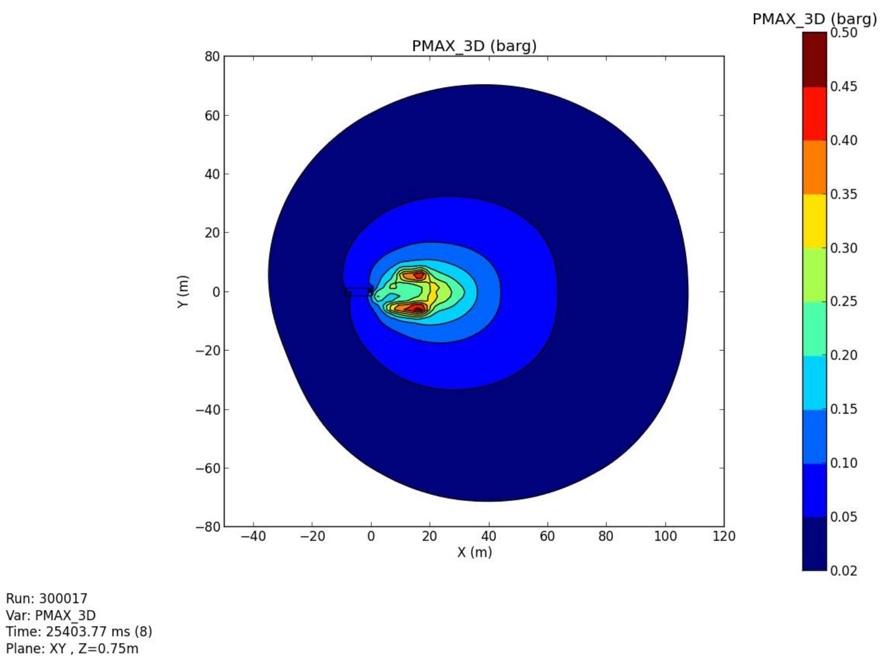


Run: 300016
Var: PMAX_3D
Time: 25411.34 ms (8)
Plane: XY , Z=0.75m

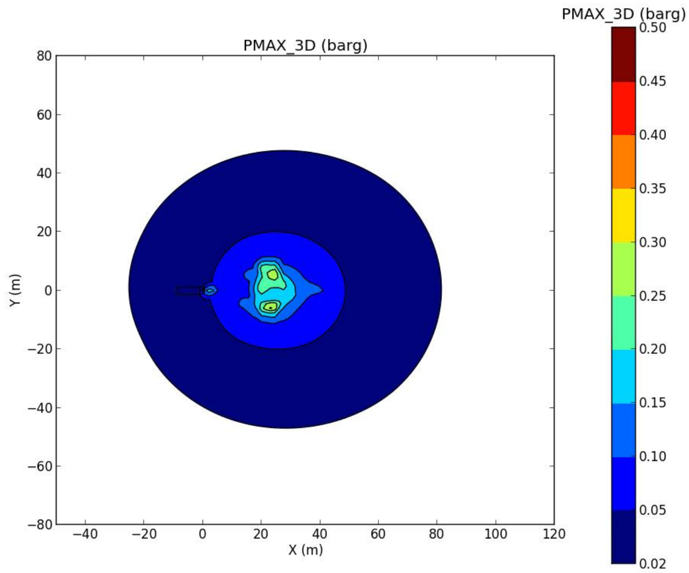
D.2. Explosion Profile at Hydrogen Concentration: 70%



D.3. Explosion Profile at Hydrogen Concentration: 67%

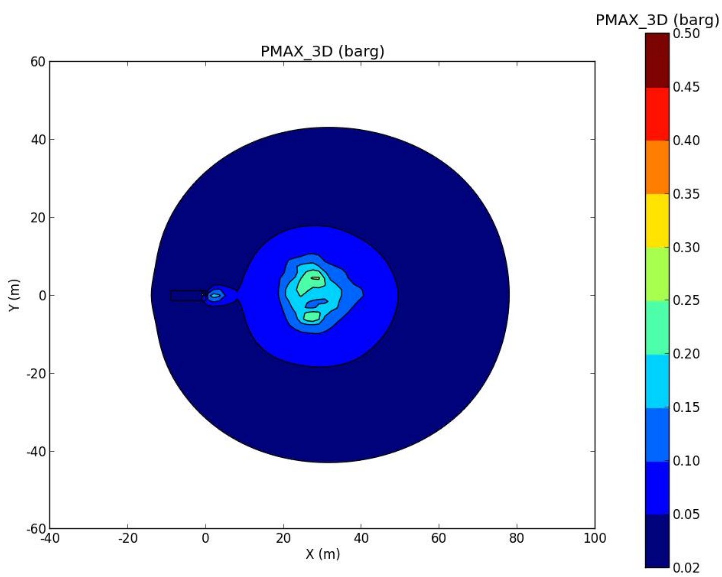


D.4. Explosion Profile at Hydrogen Concentration: 40%



Run: 300013
Var: PMAX_3D
Time: 25401.25 ms (8)
Plane: XY , Z=0.75m

D.5. Explosion Profile at Hydrogen Concentration: 36%

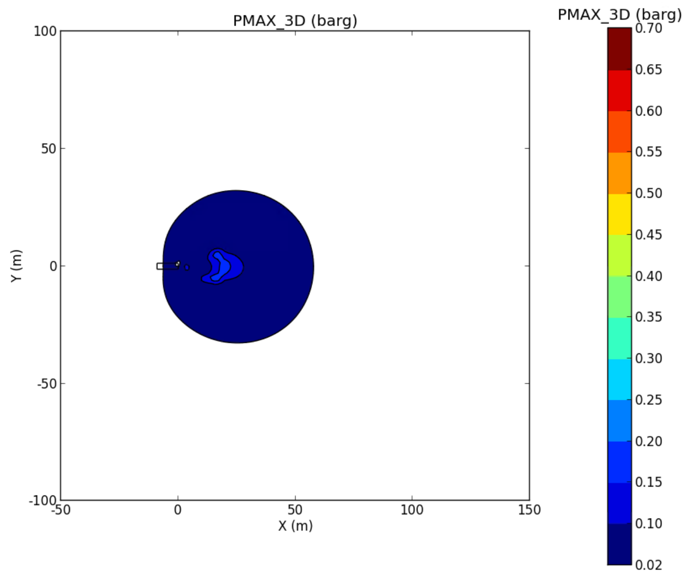


Run: 300014
Var: PMAX_3D
Time: 25394.95 ms (8)
Plane: XY , Z=0.75m

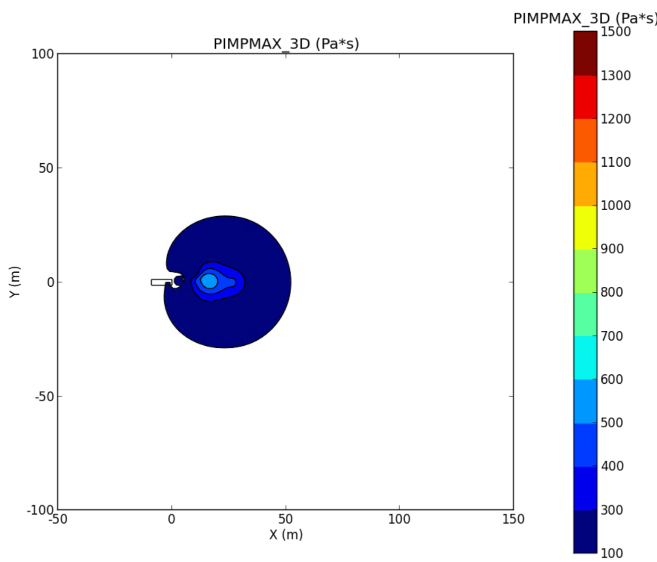
APPENDIX E

HYDROGEN EXPLOSION PROFILE

E.1. 69 bar, 1 Seconds

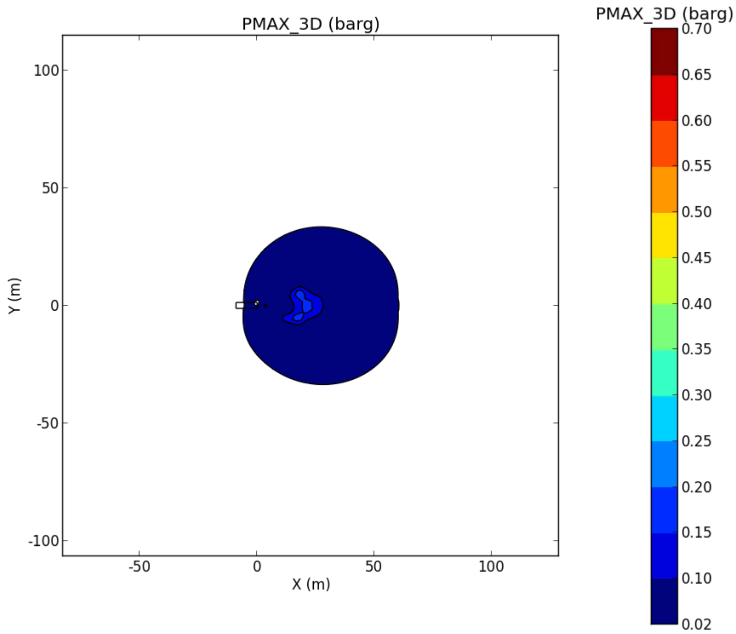


Run: 100002
Var: PMAX_3D
Time: 6.24 s (33)
Plane: XY , Z=0.75m

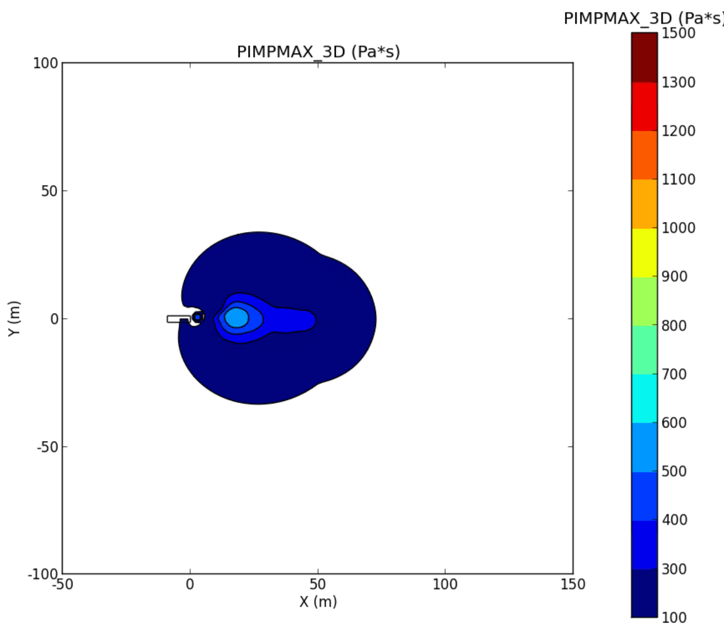


Run: 100002
Var: PIMPMAX_3D
Time: 6.24 s (33)
Plane: XY , Z=0.75m

E.2. 69 bar, 20 Seconds

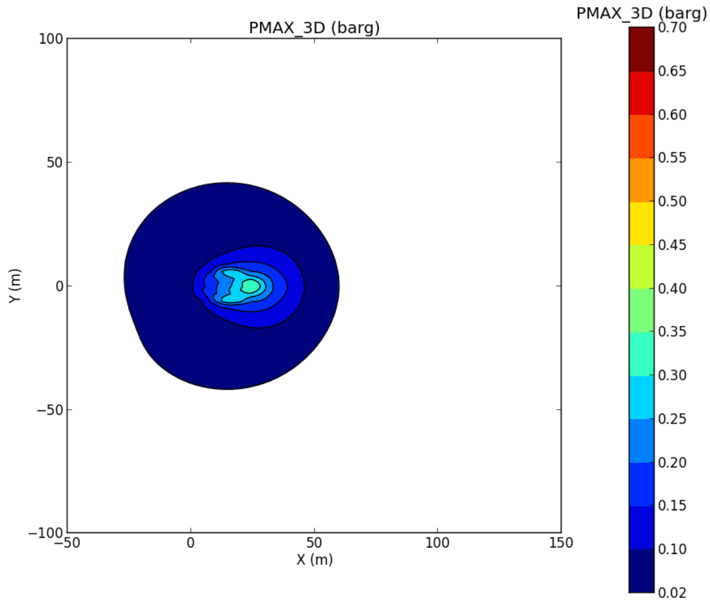


Run: 100003
Var: PMAX_3D
Time: 25.58 s (7)
Plane: XY , Z=0.75m

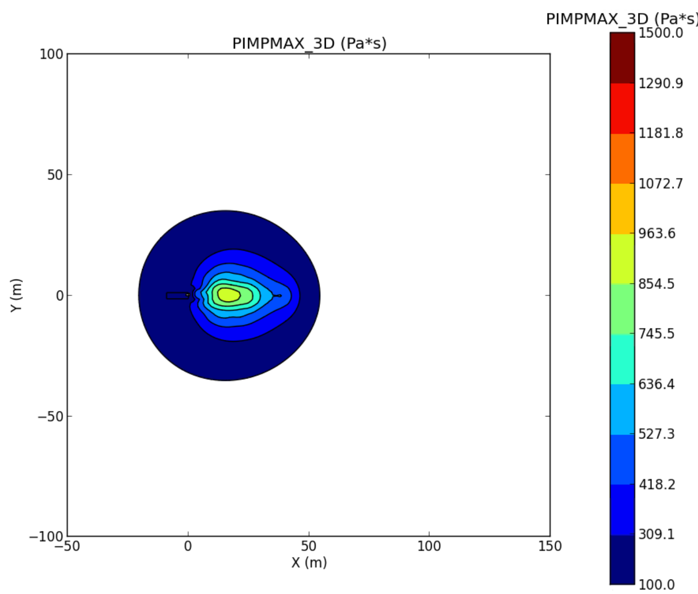


Run: 100003
Var: PIMPMAX_3D
Time: 25.48 s (6)
Plane: XY , Z=0.75m

E.3. 138 bar, 1 Seconds

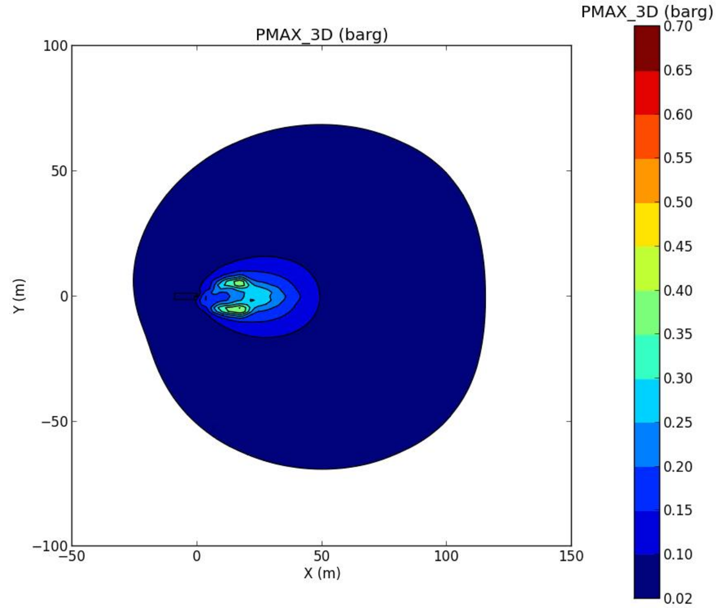


Run: 200002
Var: PMAX_3D
Time: 6.20 s (33)
Plane: XY , Z=3.75m

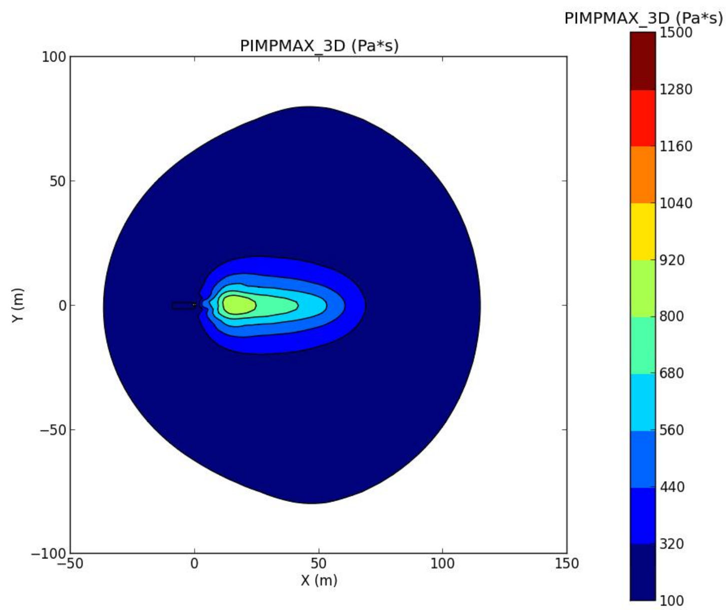


Run: 200002
Var: PIMPMAX_3D
Time: 6.20 s (33)
Plane: XY , Z=0.75m

E.4. 138 bar, 20 Seconds

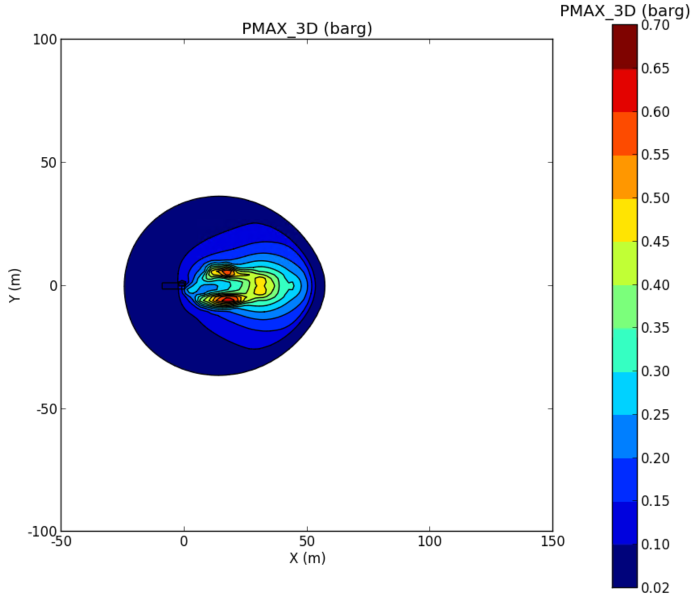


Run: 200003
Var: PMAX_3D
Time: 25.40 s (7)
Plane: XY , Z=0.75m

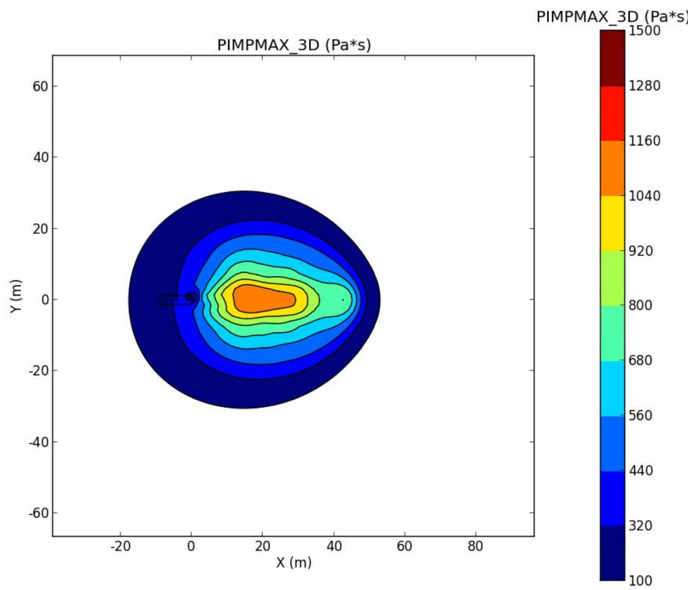


Run: 200003
Var: PIMPMAX_3D
Time: 25.40 s (7)
Plane: XY , Z=0.75m

E.5. 207 bar at 1m Height, 1 Seconds

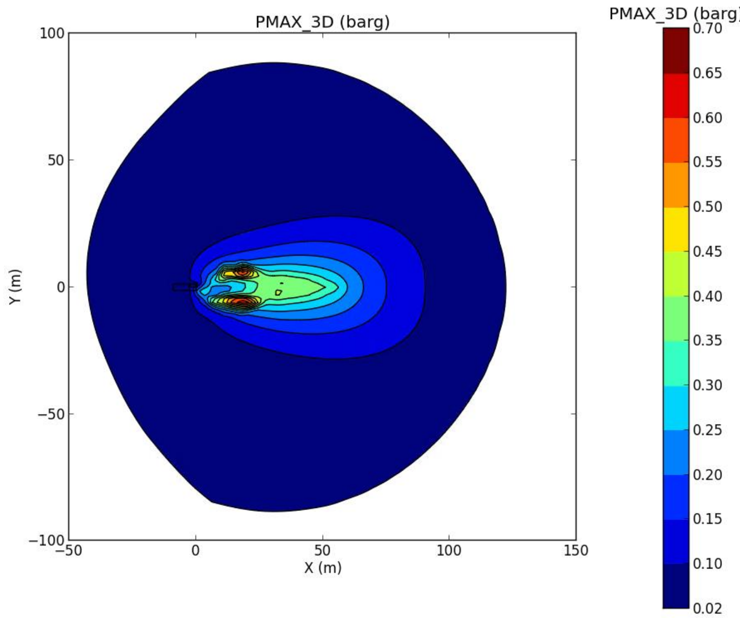


Run: 300002
Var: PMAX_3D
Time: 6.18 s (34)
Plane: XY , Z=0.75m

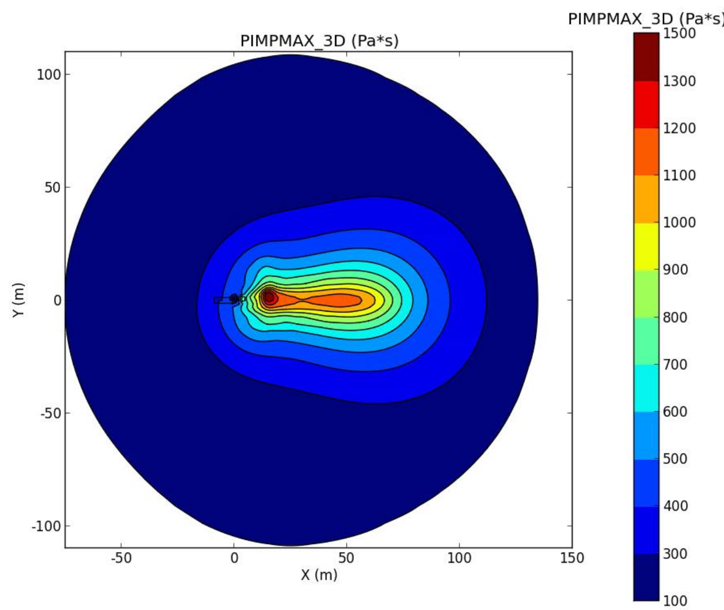


Run: 300009
Var: PIMPMAX_3D
Time: 6.18 s (34)
Plane: XY , Z=0.75m

E.6. 207 bar at 1m Height, 20 Seconds

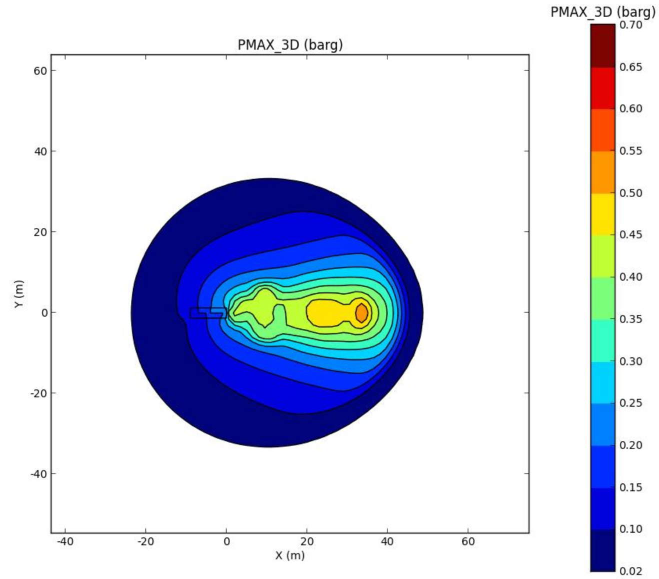


Run: 300005
Var: PMAX_3D
Time: 25.36 s (8)
Plane: XY , Z=0.75m

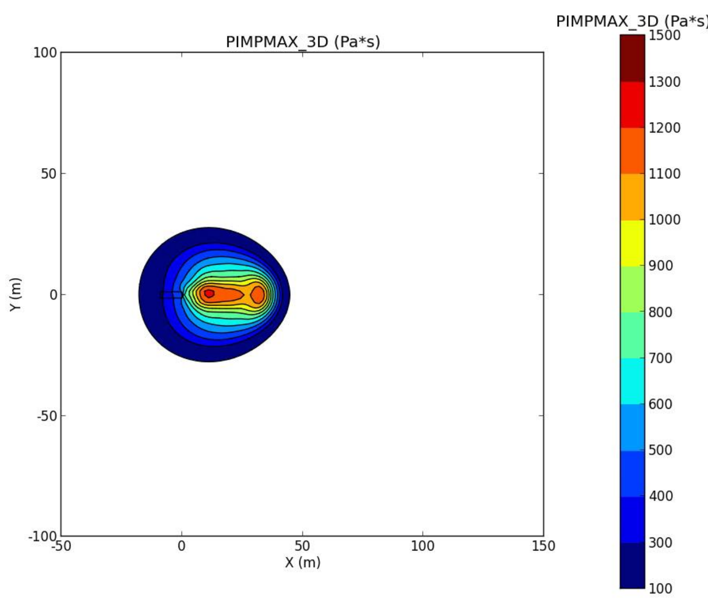


Run: 300008
Var: PIMPMAX_3D
Time: 25.43 s (9)
6 Plane: XY , Z=0.75m

E.7. 207 bar at 2 m Height, 1 Seconds



Run: 300002
Var: PMAX_3D
Time: 6150.08 ms (34)
Plane: XY , Z=0.75m



Run: 300002
Var: PIMPMAX_3D
Time: 6150.08 ms (34)
Plane: XY , Z=0.75m

E.8. 207 bar at 2 m Height, 20 Seconds